Grid Points and Generalized Discrepancies on the d-dimensional Ball

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Abstract

The problem of distributing points on a domain, like ball, plays a special role in the fields like geosciences and medical imaging. Therefore, we present an equidistribution theory with a focus on obtaining low-discrepancy point grids on a 3-dimensional ball.
The connection of the discrepancy method and the quadrature points on a given domain is quite well known. We approximate the integral of a function given on a bounded domain by the sum of function values at a specific set of points together with some weights. The idea is to get the best approximation with the fewest possible function values. The ansatz is logical, if the chosen data set is well distributed on the whole domain. This perspective, with the ball as a domain, enables us to get nice configurations as well as suitable approximations to the integrals of functions on the ball.
It is, for instance, important for choosing the centres of the radial basis functions as they are needed for regularization methods such as the RFMP algorithm and the ROFMP algorithm, developed by the Geomathematics Group at the University of Siegen for ill-posed inverse problems with particular focus on the sphere and the ball as domains of the unknown functions. Additionally, it is also important for computational purposes. For instance, for the wavelet methods with data given on the ball, where one needs to have an appropriate quadrature rule.

Zusammenfassung

Das Problem, Punkte auf einem Bereich, wie einer Kugel, zu verteilen, spielt eine wichtige Rolle in den Geowissenschaften und der medizinischen Bildgebung. Deshalb präsentieren wir eine Gleichverteilungstheorie auf der 3D-Kugel in Bezug auf Minimum-Diskrepanz-Gitter. Der Zusammenhang zwischen Diskrepanz und Punktgittern für gegebene Bereiche ist wohlbekannt. Hierbei wird das Integral einer Funktion durch eine gewichtete Summe von Funktionswerten approximiert. Die Idee besteht darin, die beste Annäherung mit möglichst wenigen Funktionswerten zu erzielen. Der Ansatz ist klar, wenn die gewählten Punkte in dem gesamten Bereich gut verteilt sind. Diese Perspektive, mit dem Ball als Bereich, ermöglicht es uns, "schöne" Strukturen sowie geeignete Näherungen an die Integrale von Funktionen auf der Kugel zu erhalten. Zum Beispiel ist es wichtig, die Mittelpunkte der radialen Basisfunktionen auszuwählen, weil diese für Regularisierungsmethoden wie den RFMP-Algorithmus und den ROFMP-Algorithmus benötigt werden. Diese Algorithmen wurden von der AG Geomathematik der Universität Siegen für schlecht gestellte inverse Probleme mit besonderem Fokus auf die Sphäre und die Kugel als Definitionsbereiche entwickelt. Darüber hinaus sind solche Gitter auch für andere numerische Zwecke hilfreich, wie z.B. für Wavelet-Verfahren auf der Kugel, die ein Quadraturgitter brauchen.

Introduction

The domain of a ball, because of its similarity with the Earth and the human brain, has always been an interesting domain for the scientists both in the fields of Earth sciences and the medical sciences. This resemblance allows and motivates us to develop more and more specific mathematical tools and techniques on the 3-dimensional ball in order to study the Earth's interior and the human brain.

At present, tomographic inverse problems have become interesting challenges for the mathematicians. For example, unprecedented data accuracies in the geosciences enable us to find out more about the Earth's interior. Long term processes in the mantle and the core of our planet can be revealed by investigating, for example, seismographic and geomagnetic data. Short-term processes at the surface which are caused, for instance, by climate change can be identified and quantified much better due to recent satellite missions. Moreover, new technologies for medical imaging open new problems of diagnostics and fundamental research. All problems of these kinds are ill-posed due to unstable solutions, i.e. small noise contained in the data usually destroys the credibility of the calculated solution, if no particular mathematical techniques such as regularization methods, are used to overcome this unstability of the data. Due to large sizes of the data sets, in particular in the geosciences and due to new requirements on the resolution of the obtained models, novel mathematical methods had to be developed. New approaches use localized basis functions —hat-like trial functions which concentrate on arbitrarily chosen regions.

For some of these new methods, the location of the hats is limited due to some traits of the methods. However, a different approach developed by the Geomathematics Group in Siegen, Germany removes this restriction and is able to deal with arbitrarily located hat functions. This method, called the RFMP algorithm has been introduced in [22, 23, 48]. This algorithm has been further dealt through different approaches and advanced versions of this algorithm that are: Regularized Orthogonal Functional Matching Pursuit (ROFMP) and Regularized Weak Functional Matching Pursuit (RWFMP)

have been developed by the Geomathematics Group Siegen. We refer the reader to [36, 37, 51, 71] for the details.
The RFMP algorithm was developed for ill-posed inverse problems with particular focus on the sphere and the ball as domains of the unknown functions. One feature of the algorithm is that it constructs a best basis out of an overcomplete selection of trial functions including, in particular, hat functions. The preprocessing of this algorithm requires that a large set of centres for the hat functions is chosen – among them a selection is made later for the best basis. In order not to impose a certain structure on the solution, it would be good to have a uniformly distributed grid for the initial large grid. Also since the interior of the Earth is composed of layers with approximately spherical boundaries, we consider the use of a cartesian grid (i.e. a tensor product grid from a 1D equidistant grid) not as an ideal choice for such applications. This arose the need for the construction of appropriate point grids together with a novel theory for the quantification of their distribution on the ball.

In this thesis, we concentrate on the construction and analysis of well distributed point grids on the ball, which includes the study of underlying Sobolev spaces as well as the construction of particular operators (pseudodifferential operators) for these spaces. In particular, we focus on the construction of low discrepancy point grids and for this we develop, implement and analyse different algorithms. The approach we used in this work is motivated by the concept given on the surface of the ball by Cui and Freeden [14]. In this thesis, we use particular orthonormal basis systems for the construction of reproducing kernel Hilbert spaces on the ball. With the help of these particular function spaces and the pseudodifferential operators, we lay down the theory of the discrepancy method. Some parts of these results have already been published in [34].
An important application of uniformly distributed grids is the use of a quadrature formula with equal weights. Since one can expect that equal quadrature weights work particularly well for equidistributed point grids, the generalized discrepancy originating from the error estimate of a quadrature formula can be used as the uniformity measure of the point grids on the ball. This perspective enables us to get nice configurations as well as suitable approximations for the integral of functions on the ball. This is useful for computational purposes, for instance, for the wavelet methods, where one needs to have an appropriate quadrature rule. We devoted a chapter (Chapter 7) in this work for this particular application of the distribution theory.
The problem of distributing points uniformly on a geomathematical surface or a domain arises, for example, in tomographic problems or as mentioned above, for approximate integration. For the case of a sphere, a lot

of research has been done in this regard. To name a few, we mention [13, 14, 31, 43, 57, 60] and the references therein. The concept of generalized discrepancy and its properties on spheres, hyperspheres and $\mathbb{R}^{d+1}$ are investigated in, for example, [3, 7, 11, 12, 13, 14, 66]. Moreover, several discrepancies are known in numerical analysis as testing tools for the distribution of a sample of points on a unit hypercube $[0,1]^d$ (see, for e.g. [10]). However, such a theory of the discrepancy method and the quadrature points on the domain of a ball is currently not known.
It should be noted that there can be different perspectives for approaching this distribution problem, as different problems may require distinct uniformity measures for the distributions which are suitable for the problem to be handled. Also, the construction of the point grids depends on the way the uniformity is measured and on the purpose for which it is required. For example, in [7] the author generates a point set on the space $\mathbb{R}^{d+1}$ with the help of Sobol points in $[0,1[^d$ and defines reproducing kernel Hilbert spaces on $\mathbb{R}^{d+1}$ as the tensor product of a reproducing kernel defined on the unit sphere Ω^d in $\mathbb{R}^{d+1}$ and a reproducing kernel defined on $[0,1[$. However, this thesis approaches the distribution problem with a different methodology and as mentioned above for handling a different problem, i.e. the regularization of ill-posed tomographic problems in the geosciences and medical imaging.

The outline of the thesis is as follows:

In Chapter 1, we lay down the mathematical foundation required for the understanding of this work. We present some basic notations and results. Specifically, we introduce classical orthogonal polynomials along with a brief summary of their properties. Moreover, complete orthonormal systems on the sphere and on the ball are introduced. We also introduce Sobolev spaces on the ball along with a smoothness condition, which tells us that these spaces possess a reproducing kernel. Since, in Chapter 5, we deal with statistical aspects of discrepancy, some statistical premilinaries are also presented in this chapter.

In Chapter 2, we present the theory of equidistribution on the ball. This idea is actually the generalization of the analogous concept on the surface of the ball given in [14].
First, we introduce the idea of pseudodifferential operators on a ball and also construct a class of such operators with the help of operators functioning on the angular and radial parts of a function. Some properties of these operators are also presented in this chapter. For example, we show that these operators are well defined and isometric. We also show that they form pseudodiffer-

ential operators with specific radial and angular orders. Further, we define particular Sobolev spaces based on the eigenvalues of these operators. These sequences of eigenvalues depend on two parameters that are related to the angular and radial parts of the function. We consider that these eigenvalues satisfy a condition due to which every function from our Sobolev space has a convergent Fourier series. This in return allows us to consider quadrature formulae with uniform and non-uniform weights and to derive estimates for the quadrature errors with some restrictions on the considered Sobolev spaces and the pseudodifferential operators in both cases. This gives us the generalized and weighted discrepancy formulae. In the end of the chapter, some representations of the discrepancy along with different operators and eigenvalues are discussed.

Chapter 3 deals with the construction of the quadrature points on the 3-dimensional ball. We consider the distribution of points on the ball out of different spherical grids via different approaches. We show how these point grids can be further modified. Moreover, we analyse these resulting configurations on the ball using the discrepancy formulae formulated in Chapter 2. The outcomes are presented in the form of plots followed by analyses about the results.

After the initial construction and modification of the point grids, we develop and investigate some algorithms for the construction of optimal or near-optimal point grids in Chapter 4. For example, we experimented with the grids by changing the maximum distance between the points or by combining a grid on the ball with a grid on the sphere. We computed the discrepancies of the resulting grids to see the effects of the algorithms. For this purpose, we also consider the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method ([29, 54]). We examine different BFGS updates and line search methods ([28, 54]) and discuss their effects on the outcomes.

In Chapter 5, some statistical aspects of discrepancy are discussed. The asymptotic properties of the generalized discrepancy for the case of a sphere are investigated by Choirat and Seri in [11]. With the help of the same concepts, we derive the properties of the generalized discrepancy on the ball. An interesting question of whether the discrepancy actually converges to zero for a uniform grid is statistically approached in this chapter. Moreover, an asymptotic distribution of the generalized discrepancy is derived.

In addition to the equidistribution theory on the 3-dimensional ball, Chapter 6 gives the generalized results for the d-dimensional case with $d \geq 3$. At first, spherical harmonics in d dimensions ([19, 53]) are briefly introduced in this chapter. Then, we construct complete orthonormal systems for higher dimensions. Further, the differential operators for these systems are derived and Sobolev spaces on a ball of d dimensions are constructed. We also present the theory of the discrepancy method and quadrature points for higher dimensions. This includes the construction of pseudodifferential operators, Sobolev spaces and the derivation of the discrepancy formula. After all this theory, the results of numerical tests for the 4-dimensional case are presented. For this purpose, we use the generalized form of a grid from Chapter 3 and the algorithms defined in Chapter 4. For the sake of brevity, two of the best algorithms are tested for the case $d = 4$. At the end of this chapter, we present some numerical properties of the generalized discrepancy. We show that the worst case error for a cubature rule is exactly the discrepancy. Further, we discuss the tractability of multivariate integration (see [55]) for our defined Sobolev spaces. A different notion of uniformity (see [3]) is discussed in the end of the chapter. Also, the convergence of the generalized discrepancy with respect to this concept is examined.

Chapter 7 presents some numerical tests in order to investigate the applicability of the equidistribution theory. Here, we deal with the numerical integration on the ball using one of the grids constructed in Chapter 3. We compute the approximate error and also the error bounds for a considered function on the ball and use the results to observe how well our grid approximates the integrals on the ball.

Finally, the outcomes of this work are summarized in Chapter 8 with some conclusions and an outlook for further research.

Contents

Chapter 1

Preliminaries

This chapter gives the basic definitions, known results and concepts for the understanding of the further work. In the first section, we introduce some general settings and the notations which we will require in this thesis. Also, we define certain function spaces on a domain $D \subset \mathbb{R}^n$ and state some established theorems (see [5, 15, 20, 38, 59, 75]). In the further sections of this chapter, we introduce briefly the orthogonal polynomials ([25, 53, 70]). Also, complete orthonormal systems on the sphere as well as on the ball are discussed along with their properties ([2, 24, 47, 50]). Furthermore, a statistical background is laid down in the last section.

1.1 Notations

In the following work, the letters $\mathbb{N}$, $\mathbb{N}_0$, $\mathbb{R}^+$, $\mathbb{R}_0^+$ and $\mathbb{C}$ denote the set of all positive integers, the set of all nonnegative integers, the set of all positive real numbers, the set of all nonnegative real numbers and the set of all complex numbers, respectively. The elements in the space $\mathbb{R}^d$ of dimension d are denoted by x, y, such that

$$x = r\xi,$$

where $r = |x|= \sqrt{x_1^2 + x_2^2 + \ldots + x_d^2}$ and $\xi = \frac{x}{|x|} \in \Omega^{d-1} := \{\eta \in \mathbb{R}^d : |\eta|= 1\}$, Ω^{d-1} denoting the $(d-1)$-sphere of radius 1. In what follows, a 2-sphere is denoted by Ω, i.e. $\Omega := \Omega^2$. A ball of radius $R \in \mathbb{R}^+$ in $\mathbb{R}^d$ is denoted and defined as

$$\mathcal{B}_R^d := \{(x_1, x_2, \ldots, x_d) \in \mathbb{R}^d : |x|\leq R\}, \quad R \in \mathbb{R}^+. \tag{1.1}$$

Specifically, a 3D unit ball and a 3D-ball of radius R are represented by $\mathcal{B}$ and $\mathcal{B}_R$, respectively.

Definition 1.1.1 *The Laplace operator in* $\mathbb{R}^3$ *is given by*

$$\Delta_x := \sum_{i=1}^{3} \frac{\partial^2}{\partial x_i^2}. \tag{1.2}$$

The polar coordinate representation of the Laplace operator is given as

$$\Delta_x = \left(\frac{\partial}{\partial r}\right)^2 + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta_\xi^*, \tag{1.3}$$

where Δ^* *is known as the Beltrami operator and is given by*

$$\Delta_\xi^* = \frac{\partial}{\partial t}\left(1-t^2\right)\frac{\partial}{\partial t} + \frac{1}{1-t^2}\left(\frac{\partial}{\partial \phi}\right)^2. \tag{1.4}$$

For $\xi \in \Omega$, *we use the following notation:*

$$\xi(\phi, t) = \begin{pmatrix} \sqrt{1-t^2}\cos\phi \\ \sqrt{1-t^2}\sin\phi \\ t \end{pmatrix},$$

where $t \in [-1, 1]$ *is the polar distance and* $\phi \in [0, 2\pi[$ *is the longitude.*

Theorem 1.1.2 *The gradient* ∇ *in* $\mathbb{R}^3$ *can be written as the sum of a radial and an angular part, i.e.*

$$\nabla = \varepsilon^r \frac{\partial}{\partial r} + \frac{1}{r}\nabla^*, \tag{1.5}$$

where ∇^* *is the surface gradient given by*

$$\nabla^* := \varepsilon^\phi \frac{1}{\sqrt{1-t^2}}\frac{\partial}{\partial \phi} + \varepsilon^t \sqrt{1-t^2}\frac{\partial}{\partial t}, \tag{1.6}$$

with orthonormal vectors

$$\begin{aligned} \varepsilon^r(\phi, t) &:= \xi, \quad \xi \in \Omega \\ \varepsilon^\phi(\phi) &:= \begin{pmatrix} -\sin\phi \\ \cos\phi \\ 0 \end{pmatrix}, \\ \varepsilon^t(\phi, t) &:= \begin{pmatrix} t\cos\phi \\ t\sin\phi \\ \sqrt{1-t^2} \end{pmatrix}. \end{aligned}$$

Definition 1.1.3 *For any $x > 0$, the gamma function of x is denoted by $\Gamma(x)$ and is defined as*

$$\Gamma(x) := \int_0^\infty e^{-t} t^{x-1} \mathrm{d}t,$$

with

$$\Gamma(x+1) = x\Gamma(x), \quad x > 0 \tag{1.7}$$

and

$$\Gamma(n+1) = n!\,, \quad n \in \mathbb{N}_0. \tag{1.8}$$

Lemma 1.1.4 (Duplication Formula). *For $x > 0$, we have*

$$2^{x-1}\Gamma\left(\frac{x}{2}\right)\Gamma\left(\frac{x+1}{2}\right) = \sqrt{\pi}\,\Gamma(x). \tag{1.9}$$

Definition 1.1.5 *For all x, $y > 0$, the beta function $(x, y) \mapsto \mathrm{B}(x, y)$ is defined as*

$$\mathrm{B}(x, y) := \int_0^1 t^{x-1}(1-t)^{y-1}\mathrm{d}t = \int_0^\infty \frac{t^{x-1}}{(1+t)^{x+y}}\,\mathrm{d}t. \tag{1.10}$$

Theorem 1.1.6 *Let B and Γ be the functions as defined above, then*

$$\mathrm{B}(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$$

for all x, $y > 0$.

Definition 1.1.7 *For r, $k \in \mathbb{N}_0$ with $k \le r$, the binomial coefficients in terms of gamma functions are defined by*

$$\binom{r}{k} := \frac{\Gamma(r+1)}{\Gamma(k+1)\Gamma(r-k+1)}. \tag{1.11}$$

We mention here some of the properties of binomial coefficients from [30].

Theorem 1.1.8 *The binomial coefficients have the following properties:*

1. *Binomial products: For $r \ge n \ge k \ge 0$,*

$$\binom{r}{n}\binom{n}{k} = \binom{r}{k}\binom{r-k}{n-k}. \tag{1.12}$$

2. *Sum of binomial products (also known as Vandermonde's identity): For* X, $Y > 0$ *and* $n \in \mathbb{N}_0$,

$$\sum_{k=0}^{n} \binom{X}{k}\binom{Y}{n-k} = \binom{X+Y}{n}. \tag{1.13}$$

3. *Negating the upper index of a binomial coefficient: For* r, $k \in \mathbb{N}_0$ *with* $k - r - 1 > 0$,

$$\binom{r}{k} = (-1)^k \binom{k-r-1}{k}. \tag{1.14}$$

Remark 1.1.9 **([30])**. *The above identities are also valid for all* $r \in \mathbb{R}$.

Definition 1.1.10 *The symbol* δ_{ij} *represents the Kronecker delta and is given as*

$$\delta_{ij} := \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

Definition 1.1.11 *Let* F *and* G *be two univariate functions and* $x_0 \in \mathbb{R} \cup \{-\infty, +\infty\}$, *then the Landau symbol* $\mathcal{O}$ *is defined as*

$$F(x) = \mathcal{O}\left(G(x)\right) \text{ as } x \to x_0 \text{ if and only if } \frac{F(x)}{G(x)} \text{ is bounded as } x \to x_0$$

and the symbol o *is defined as*

$$F(x) = o\left(G(x)\right) \text{ as } x \to x_0 \text{ if and only if } \lim_{x \to x_0} \frac{F(x)}{G(x)} = 0.$$

Definition 1.1.12 *A Pre-Hilbert space* X *is a nonempty real vector space together with an inner product*

$$\langle \cdot, \cdot \rangle : X \times X \to \mathbb{R},$$

satisfying the following properties for all x, y, $z \in X$ *and* λ, $\mu \in \mathbb{R}$:

(i) $\langle x, x \rangle \geq 0$.

(ii) $\langle x, x \rangle = 0$ *if and only if* $x = 0$.

(iii) $\langle x, y \rangle = \langle y, x \rangle$.

(iv) $\langle \lambda x + \mu y, z \rangle = \lambda \langle x, z \rangle + \mu \langle y, z \rangle$.

Remark 1.1.13 *A complete Pre-Hilbert space is called a Hilbert space.*

Definition 1.1.14 *A Hilbert space H of functions on a domain $D \subset \mathbb{R}^n$ is said to be a reproducing kernel Hilbert space if there exists a kernel $K_H : D \times D \to \mathbb{R}$ satisfying the following properties:*

1. $K_H(x, \cdot) \in H$ *for all* $x \in D$.

2. $\langle K_H(x, \cdot), F \rangle = F(x)$ *for all* $x \in D$ *and for all* $F \in H$.

Definition 1.1.15 *Let H be a Hilbert space of real valued functions F on a domain D. For a fixed $x \in D$, the map*

$$\begin{aligned} \mathcal{L}_x : H &\to \mathbb{R} \\ F &\mapsto F(x) \end{aligned}$$

is called the evaluation functional at x.

Theorem 1.1.16 (Aronszajn's Theorem). *The Hilbert space H of functions on $D \subset \mathbb{R}^n$ is a reproducing kernel Hilbert space if and only if the evaluation functional $\mathcal{L}_x$ is continuous for each $x \in D$.*

Theorem 1.1.17 *For a reproducing kernel Hilbert space H of functions on $D \subset \mathbb{R}^n$ the corresponding reproducing kernel K_H is uniquely represented by*

$$K_H(x, y) = \sum_{k=0}^{\infty} U_k(x) U_k(y) \quad \text{for all } x, y \in D, \tag{1.15}$$

given that $\{U_k\}_{k \in \mathbb{N}_0}$ is a complete orthonormal system in H satisfying

$$\sum_{k=0}^{\infty} U_k(x)^2 < +\infty \quad \text{for all } x \in D. \tag{1.16}$$

Theorem 1.1.18 ([15]). *Let H be a Hilbert space of functions on a domain $D \subset \mathbb{R}^n$ and $\mathcal{L} : H \to \mathbb{R}$ be a bounded linear functional on the Hilbert space H. Then,*

1. *the function* $D \ni y \mapsto \mathcal{L}_x K_H(x, y)$ *is an element of* H.

2. $\mathcal{L}(F) = \langle F, \mathcal{L}_x K_H(x, \cdot) \rangle_H$ *for all* $F \in H$.

Definition 1.1.19 *A vector space X together with a mapping (called norm)*

$$\|\cdot\| : X \to \mathbb{R},$$

is named as a normed space if for all x, $y \in X$, the following holds:

(i) $\|x\| \geq 0$.

(ii) $\|x\| = 0$ *if and only if* $x = 0$.

(iii) $\|\lambda x\| = |\lambda| \|x\|$ *for all* $\lambda \in \mathbb{R}$.

(iv) $\|x + y\| \leq \|x\| + \|y\|$.

Remark 1.1.20 *Every pre-Hilbert space* X *is a normed space with norm*

$$\|x\| = \sqrt{\langle x, x \rangle} \quad \text{for all } x \in X.$$

It is called the induced norm.

Theorem 1.1.21 (Cauchy-Schwarz Inequality). *An inner product with the corresponding induced norm on the space* X *satisfies the Cauchy-Schwarz inequality, i.e. for all* x, $y \in X$

$$|\langle x, y \rangle| \leq \|x\| \|y\|. \tag{1.17}$$

Definition 1.1.22 *Let* $D \subset \mathbb{R}^n$ *be compact. Then* $\mathrm{C}^k(D)$ *denotes the space of all functions* $F : D \to \mathbb{R}^m$ *on* D *possessing* k *continuous derivatives. In particular,* $\mathrm{C}^0(D) := \mathrm{C}(D)$ *is a complete normed space with the norm*

$$\|F\|_{\mathrm{C}(D)} := \max_{x \in D} |F(x)|.$$

Definition 1.1.23 *Let* $D \subset \mathbb{R}^n$ *be a Lebesgue measurable space with* $1 \leq p < +\infty$. *Let* $\mathcal{L}^p(D)$ *be the space of all measurable functions* $F : D \to \mathbb{R}$ *that satisfy*

$$\int_D |F(x)|^p \, \mathrm{d}x < +\infty$$

and $\mathcal{N}^p(D)$ *denote the space of all measurable functions* $F : D \to \mathbb{R}$ *with*

$$\int_D |F(x)|^p \, \mathrm{d}x = 0.$$

Then the normed space $(\mathrm{L}^p(D), \|\cdot\|_p)$ *is defined by*

$$\mathrm{L}^p(D) := \mathcal{L}^p(D) / \mathcal{N}^p(D)$$

with the norm

$$\|F\|_{\mathrm{L}^p(D)} := \left(\int_D |F(x)|^p \, \mathrm{d}x \right)^{\frac{1}{p}}. \tag{1.18}$$

In particular, for the case of $p = 2$, $\mathrm{L}^2(D)$ *forms a Hilbert space with the inner product*

$$\langle F, G \rangle_{\mathrm{L}^2(D)} := \int_D F(x) G(x) \mathrm{d}x. \tag{1.19}$$

Definition 1.1.24 *Let* $w \in \mathrm{C}[a,b]$ *with* $w > 0$ *in* (a,b)*. Further, let* $\mathcal{L}^2_w[a,b]$ *be the space of all measurable functions* $F : [a,b] \to \mathbb{R}$ *that satisfy*

$$\int_a^b F(x)^2 w(x)\,\mathrm{d}x < +\infty$$

and $\mathcal{N}^2_w[a,b]$ *denote the space of all measurable functions* $F : [a,b] \to \mathbb{R}$ *with*

$$\int_a^b F(x)^2 w(x)\,\mathrm{d}x = 0.$$

Then the Hilbert space $\left(\mathrm{L}^2_w[a,b], \langle\cdot,\cdot\rangle_{\mathrm{L}^2_w[a,b]}\right)$ *is defined by*

$$\mathrm{L}^2_w[a,b] := \mathcal{L}^2_w[a,b]/\mathcal{N}^2_w[a,b]$$

with the inner product

$$\langle F, G\rangle_{\mathrm{L}^2_w[a,b]} := \int_a^b F(x)G(x)w(x)\,\mathrm{d}x. \tag{1.20}$$

The substitution rule for volume integrals leads us to the following theorem.

Theorem 1.1.25 *Let* $0 \leq a < b < +\infty$ *and* $D := \{x \in \mathbb{R}^3 \,|\, a \leq |x| \leq b\}$*, then*

$$\int_D F(x)\mathrm{d}x = \int_a^b r^2 \int_\Omega F(r\xi)\,\mathrm{d}\omega(\xi)\,\mathrm{d}r \tag{1.21}$$

for all $F \in \mathrm{C}(D)$*, provided that the integrals exist.*

Theorem 1.1.26 (Uniform Convergence Theorem). *If* $\{f_n\}_{n\in\mathbb{N}_0}$ *is a sequence of continuous functions defined on a domain* D *that converges uniformly to the function* f *on* D*, then* f *is also continuous on* D*.*

Theorem 1.1.27 (Dini's Theorem). *Let* $D \subset \mathbb{R}^n$ *be compact, and*

(i) $\{f_n\}_{n\in\mathbb{N}_0}$ *be a sequence of continuous functions on* D*,*

(ii) $\{f_n\}_{n\in\mathbb{N}_0}$ *converge pointwise to a continuous function* f *on* D*,*

(iii) $\{f_n\}_{n\in\mathbb{N}_0}$ *be monotonic.*

Then, $\{f_n\}_{n\in\mathbb{N}_0}$ *converges uniformly to* f *on* D*.*

Definition 1.1.28 *A subset* S *of a pre-Hilbert space* X *is called an orthogonal set if all its elements are pairwise orthogonal, i.e. for all* $x, y \in S$

$$\langle x, y\rangle = 0, \qquad \text{if } x \neq y.$$

Definition 1.1.29 *A subset S of a pre-Hilbert space X is known as an orthonormal set if for all x, $y \in S$,*

$$\langle x, y \rangle = \begin{cases} 0, & \text{if } x \neq y, \\ 1, & \text{if } x = y. \end{cases}$$

In the case of a countable system $\{x_n\}_{n\in\mathbb{N}_0}$, we can say that it is orthonormal if

$$\langle x_n, x_m \rangle = \delta_{nm}, \quad n, m \in \mathbb{N}_0. \tag{1.22}$$

Theorem 1.1.30 *For an orthonormal system $\{x_n\}_{n\in\mathbb{N}_0}$ in a Hilbert space H, the following properties are equivalent:*

1. *$\{x_n\}_{n\in\mathbb{N}_0}$ is complete, i.e. for $F \in H$*

$$\text{if } \langle F, x_n \rangle_H = 0 \text{ for all } n \in \mathbb{N}, \text{ then } F = 0. \tag{1.23}$$

2. *$H = \overline{\operatorname{span}\{x_n \,|\, n \in \mathbb{N}_0\}}^{\|\cdot\|}$.*

3. *Every element $F \in H$ can be expanded as a Fourier series, i.e.*

$$F = \sum_{n\in\mathbb{N}_0} \langle F, x_n \rangle_H \, x_n. \tag{1.24}$$

4. *The Parseval identities hold:*

$$\|F\|_H^2 = \sum_{n\in\mathbb{N}_0} \langle F, x_n \rangle_H^2, \tag{1.25}$$

$$\langle F, G \rangle_H = \sum_{n\in\mathbb{N}_0} \langle F, x_n \rangle_H \langle G, x_n \rangle_H \tag{1.26}$$

for all $F, G \in H$.

1.2 Orthogonal Polynomials

This section gives the details about the classical orthogonal polynomials, known as Jacobi polynomials, and some particular cases of these polynomials. We also state their properties that will be required later. For details, the reader is referred to [1, 9, 44, 70].

Definition 1.2.1 *For $n \in \mathbb{N}_0$, $\alpha, \beta > -1$, the functions $P_n^{(\alpha,\beta)}$ defined on the interval $[-1, 1]$, are named as **Jacobi polynomials**, if they satisfy the following properties:*

1. $\deg P_n^{(\alpha,\beta)} = n$.
2. *For weights* $w(x) = (1-x)^\alpha(1+x)^\beta$,
$$\int_{-1}^{1} w(x)P_m^{(\alpha,\beta)}(x)P_n^{(\alpha,\beta)}(x)\mathrm{d}x = 0 \quad \textit{for } n \neq m. \tag{1.27}$$
3. $P_n^{(\alpha,\beta)}(1) = \frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)}$.

Theorem 1.2.2 *For* $w \in \mathrm{C}[-1,1]$ *with* $w(x) = (1-x)^\alpha(1+x)^\beta$, *where* $w > 0$ *in* $(-1,1)$ *and a sequence* $\binom{n+\alpha}{n}$ *with* $n \in \mathbb{N}_0$, *Jacobi polynomials are the only polynomials that are determined by the properties in Definition 1.2.1.*

Theorem 1.2.3 *The Jacobi polynomials* $y = P_n^{(\alpha,\beta)}$ *satisfy the following second order, linear, homogeneous differential equation:*

$$\left(1-x^2\right)\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + (\beta-\alpha-(\alpha+\beta+2)x)\frac{\mathrm{d}y}{\mathrm{d}x} + n(n+\alpha+\beta+1)y = 0. \tag{1.28}$$

Theorem 1.2.4 (Rodriguez Formula). *For* α, $\beta > -1$, $n \in \mathbb{N}_0$ *and for all* $x \in [-1,1]$, *the Jacobi polynomials* $P_n^{(\alpha,\beta)}$ *satisfy*

$$(1-x)^\alpha(1+x)^\beta P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n n!}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n\left((1-x)^{n+\alpha}(1+x)^{n+\beta}\right). \tag{1.29}$$

We mention here another representation of Jacobi polynomials (see [70]). For α, $\beta > -1$ and $n \in \mathbb{N}_0$, we have

$$\begin{aligned} &P_n^{(\alpha,\beta)}(x) \\ &= \frac{1}{n!}\sum_{\nu=0}^{n}\binom{n}{\nu}(n+\alpha+\beta+1)\ldots(n+\alpha+\beta+\nu)(\alpha+\nu+1)\ldots(\alpha+n)\left(\frac{x-1}{2}\right)^\nu, \end{aligned}$$

which can be rewritten as

$$P_n^{(\alpha,\beta)}(x) = \sum_{\nu=0}^{n}\binom{n+\alpha+\beta+\nu}{\nu}\binom{n+\alpha}{n-\nu}\left(\frac{x-1}{2}\right)^\nu. \tag{1.30}$$

Now, we state the following result from [27] (Proposition 2.6) for our required settings.

Theorem 1.2.5 *Let* $x = 2r^2 - 1$ *with* $r \in [0,1]$, *then*

$$\left(r^2-1\right)^\alpha P_n^{(\alpha,\beta)}\left(2r^2-1\right) = \sum_{k=0}^{\alpha+n}(-1)^{\alpha+n-k}\binom{\alpha+n}{k}\binom{\beta+k+n}{n}r^{2k} \tag{1.31}$$

for all $\alpha \in \mathbb{N}_0$ *and* $\beta > -1$.

Proof: Substituting $x = 2r^2 - 1$ in equation (1.30), we get

$$P_n^{(\alpha,\beta)}\left(2r^2-1\right) = \sum_{\nu=0}^{n} \binom{n+\alpha+\beta+\nu}{\nu}\binom{n+\alpha}{n-\nu}\left(r^2-1\right)^{\nu}.$$

Further, multiplying both sides by the term $(r^2-1)^{\alpha}$ and using the binomial expansion, the above equation takes the form

$$\begin{aligned}
&\left(r^2-1\right)^{\alpha} P_n^{(\alpha,\beta)}\left(2r^2-1\right)\\
&= \sum_{\nu=0}^{n} \binom{n+\alpha+\beta+\nu}{\nu}\binom{n+\alpha}{n-\nu}\left(r^2-1\right)^{\alpha+\nu}\\
&= \sum_{\nu=0}^{n} \binom{n+\alpha+\beta+\nu}{\nu}\binom{n+\alpha}{n-\nu}\sum_{k=0}^{\alpha+\nu}(-1)^{\alpha+\nu-k}\binom{\alpha+\nu}{k}(r^2)^k\\
&= \sum_{\nu=0}^{n} \binom{n+\alpha+\beta+\nu}{\nu}\binom{n+\alpha}{\alpha+\nu}\sum_{k=0}^{\alpha+\nu}(-1)^{\alpha+\nu-k}\binom{\alpha+\nu}{k}r^{2k}. \qquad (1.32)
\end{aligned}$$

With the help of property (1.12), we can write

$$\begin{aligned}
\binom{n+\alpha}{\alpha+\nu}\binom{\alpha+\nu}{k} &= \binom{n+\alpha}{k}\binom{n+\alpha-k}{\alpha+\nu-k}\\
&= \binom{n+\alpha}{k}\binom{n+\alpha-k}{n-\nu}. \qquad (1.33)
\end{aligned}$$

Inserting (1.33) in (1.32), we arrive at

$$\begin{aligned}
&\left(r^2-1\right)^{\alpha} P_n^{(\alpha,\beta)}\left(2r^2-1\right)\\
&= \sum_{\nu=0}^{n} \binom{n+\alpha+\beta+\nu}{\nu}\sum_{k=0}^{\alpha+\nu}(-1)^{\alpha+\nu-k}\binom{n+\alpha}{k}\binom{n+\alpha-k}{n-\nu}r^{2k}.
\end{aligned}$$

Now, changing the order of summation and using (1.14), i.e.

$$(-1)^{\nu}\binom{n+\alpha+\beta+\nu}{\nu} = \binom{-n-\alpha-\beta-1}{\nu},$$

we get

$$\begin{aligned}
&\left(r^2-1\right)^{\alpha} P_n^{(\alpha,\beta)}\left(2r^2-1\right)\\
&= \sum_{k=0}^{\alpha+n}(-1)^{\alpha-k}\binom{\alpha+n}{k}r^{2k}\sum_{\nu=0}^{n}\binom{-n-\alpha-\beta-1}{\nu}\binom{n+\alpha-k}{n-\nu}.
\end{aligned}$$

From Vandermonde's identity (1.13), we know that

$$\sum_{\nu=0}^{n} \binom{-n-\alpha-\beta-1}{\nu} \binom{n+\alpha-k}{n-\nu} = \binom{-\beta-k-1}{n}.$$

Again using (1.14), we get

$$\binom{-\beta-k-1}{n} = (-1)^n \binom{\beta+k+n}{n}.$$

By virtue of the above considerations, we finally get

$$\left(r^2-1\right)^{\alpha} P_n^{(\alpha,\beta)}\left(2r^2-1\right) = \sum_{k=0}^{\alpha+n} (-1)^{\alpha+n-k} \binom{\alpha+n}{k} \binom{\beta+k+n}{n} r^{2k},$$

as required. ■

Remark 1.2.6 *For $\alpha = 0$,* (1.31) *becomes*

$$P_n^{(0,\beta)}\left(2r^2-1\right) = \sum_{k=0}^{n} (-1)^{n-k} \binom{n}{k} \binom{\beta+k+n}{n} r^{2k}. \tag{1.34}$$

The Jacobi polynomials can be easily calculated using the following three-term recurrence relation.

Theorem 1.2.7 (Recurrence Formula). *For every α, $\beta > -1$ and $x \in [-1,1]$, the Jacobi polynomials are given by*

$$\begin{aligned}
&P_0^{(\alpha,\beta)}(x) = 1,\\
&P_1^{(\alpha,\beta)}(x) = \frac{1}{2}(\alpha+\beta+2)x + \frac{1}{2}(\alpha-\beta),\\
&P_n^{(\alpha,\beta)}(x)\\
&\quad = \frac{(2n+\alpha+\beta-1)[(2n+\alpha+\beta)(2n+\alpha+\beta-2)x+\alpha^2-\beta^2]}{2n(n+\alpha+\beta)(2n+\alpha+\beta-2)} P_{n-1}^{(\alpha,\beta)}(x)\\
&\qquad - \frac{2(n+\alpha-1)(n+\beta-1)(2n+\alpha+\beta)}{2n(n+\alpha+\beta)(2n+\alpha+\beta-2)} P_{n-2}^{(\alpha,\beta)}(x), \quad n \geq 2.
\end{aligned}$$

Theorem 1.2.8 *For $n \in \mathbb{N}_0$, $\alpha, \beta > -1$, the k-th derivative of $P_n^{(\alpha,\beta)}$ is given as*

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k} P_n^{(\alpha,\beta)}(x) = \frac{\Gamma(\alpha+\beta+n+k+1)}{2^k \Gamma(\alpha+\beta+n+1)} P_{n-k}^{(\alpha+k,\beta+k)}(x). \tag{1.35}$$

The Jacobi polynomials are reduced to some particular cases for different values of α and β. Here, we will discuss two of the cases, which will be used later in the work.

1. For $\alpha = \beta$, Jacobi polynomials are reduced to **Gegenbauer polynomials**, also known as **ultraspherical polynomials**. They are related to the general Jacobi polynomials by the following equation:

$$\begin{aligned} C_n^{\lambda}(x) &= \frac{\Gamma(\alpha+1)\Gamma(n+2\alpha+1)}{\Gamma(2\alpha+1)\Gamma(n+\alpha+1)} P_n^{(\alpha,\alpha)}(x) \\ &= \frac{\Gamma(\lambda+\frac{1}{2})\Gamma(n+2\lambda)}{\Gamma(2\lambda)\Gamma(n+\lambda+\frac{1}{2})} P_n^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}(x), \end{aligned} \tag{1.36}$$

where $\lambda \neq 0$ and $\alpha = \beta = \lambda - \frac{1}{2}$, $\lambda > -\frac{1}{2}$. Using Theorem 1.2.4, we can derive the Rodriguez formula for the Gegenbauer polynomials as follows: For $\alpha = \beta = \lambda - \frac{1}{2}$, equation (1.29) gives

$$\left(1-x^2\right)^{\lambda-\frac{1}{2}} P_n^{\left(\lambda-\frac{1}{2},\lambda-\frac{1}{2}\right)}(x) = \frac{(-1)^n}{2^n n!} \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(1-x^2\right)^{n+\lambda-\frac{1}{2}}.$$

Next, multiplying both sides by the term $\frac{\Gamma(\lambda+\frac{1}{2})\Gamma(n+2\lambda)}{\Gamma(2\lambda)\Gamma(n+\lambda+\frac{1}{2})}$ and using the relation (1.36), we get

$$\left(1-x^2\right)^{\lambda-\frac{1}{2}} C_n^{\lambda}(x) = \frac{(-1)^n}{2^n n!} \frac{\Gamma(\lambda+\frac{1}{2})\Gamma(n+2\lambda)}{\Gamma(2\lambda)\Gamma(n+\lambda+\frac{1}{2})} \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(1-x^2\right)^{n+\lambda-\frac{1}{2}}.$$

This gives us the following representation for the Gegenbauer polynomials:

$$C_n^{\lambda}(x) = \frac{(-1)^n \Gamma(\lambda+\frac{1}{2})\Gamma(n+2\lambda)}{2^n n!\, \Gamma(2\lambda)\Gamma(n+\lambda+\frac{1}{2})} \left(1-x^2\right)^{\frac{1}{2}-\lambda} \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(1-x^2\right)^{n+\lambda-\frac{1}{2}}.$$

Further, we formulate the corresponding three-term recurrence relation using Theorem 1.2.7 with $\alpha = \beta = \lambda - \frac{1}{2}$ and the relation (1.36). It is easy to see that for $n = 0$ and $n = 1$ with

$$P_0^{\left(\lambda-\frac{1}{2},\lambda-\frac{1}{2}\right)}(x) = 1 \quad \text{and} \quad P_1^{\left(\lambda-\frac{1}{2},\lambda-\frac{1}{2}\right)}(x) = \left(\lambda + \frac{1}{2}\right) x,$$

we have

$$C_0^{\lambda}(x) = 1 \quad \text{and} \quad C_1^{\lambda}(x) = 2\lambda x.$$

For $n \geq 2$, we multiply the recurrence formula for Jacobi polynomials by the term $\frac{\Gamma(\lambda+\frac{1}{2})\Gamma(n+2\lambda)}{\Gamma(2\lambda)\Gamma(n+\lambda+\frac{1}{2})}$ and use the relation (1.36) to get

$$\begin{aligned} C_n^\lambda(x) = {} & \frac{(n+\lambda-1)(2n+2\lambda-1)(2n+2\lambda-3)x}{n(2n+2\lambda-3)(n+\lambda-\frac{1}{2})} \\ & \times \frac{\Gamma(\lambda+\frac{1}{2})\Gamma(n+2\lambda-1)}{\Gamma(2\lambda)\Gamma(n+\lambda-\frac{1}{2})} P_{n-1}^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}(x) \\ & - \frac{(n+\lambda-\frac{3}{2})(2n+2\lambda-1)(n+2\lambda-2)}{n(2n+2\lambda-3)(n+\lambda-\frac{1}{2})} \\ & \times \frac{\Gamma(\lambda+\frac{1}{2})\Gamma(n+2\lambda-2)}{\Gamma(2\lambda)\Gamma(n+\lambda-\frac{3}{2})} P_{n-2}^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}(x) \\ = {} & \frac{(n+\lambda-1)(2n+2\lambda-1)(2n+2\lambda-3)x}{n(2n+2\lambda-3)(n+\lambda-\frac{1}{2})} C_{n-1}^\lambda(x) \\ & - \frac{(n+\lambda-\frac{3}{2})(2n+2\lambda-1)(n+2\lambda-2)}{n(2n+2\lambda-3)(n+\lambda-\frac{1}{2})} C_{n-2}^\lambda(x). \end{aligned}$$

Some easy simplifications gives us the following relation for Gegenbauer polynomials:

$$nC_n^\lambda(x) = 2(n+\lambda-1)xC_{n-1}^\lambda(x) - (n+2\lambda-2)C_{n-2}^\lambda(x), \quad n \geq 2, \tag{1.37}$$

with $C_0^\lambda(x) = 1$ and $C_1^\lambda(x) = 2\lambda x$.

2. For $\alpha = \beta = 0$, we get the **Legendre polynomials** $P_n := P_n^{(0,0)}$. Using Theorem 1.2.4, the Rodriguez representation for the Legendre polynomials is given by

$$P_n(x) = \frac{(-1)^n}{2^n n!} \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(1-x^2\right)^n.$$

And by virtue of Theorem 1.2.7, the corresponding three-term recurrence relation is given as

$$P_n(x) = \frac{2n-1}{n} x P_{n-1}(x) - \frac{n-1}{n} P_{n-2}(x), \quad n \geq 2,$$

with $P_0(x) = 1$ and $P_1(x) = x$.

Theorem 1.2.9 *For $n \in \mathbb{N}$ and $\lambda \neq 0$, the k-th derivative of Gegenbauer polynomials is given as*

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k} C_n^\lambda(x) = 2^k \lambda^k C_{n-k}^{\lambda+k}(x). \tag{1.38}$$

Theorem 1.2.10 *For $\alpha, \beta > -1$, we have*

$$\max_{-1\le x\le 1} \left|P_n^{(\alpha,\beta)}(x)\right| = \binom{n+q}{n},$$

where $q = \max(\alpha, \beta) \ge -\frac{1}{2}$. In particular, for $\alpha = \beta = \lambda - \frac{1}{2}$, $\lambda > 0$

$$\max_{-1\le x\le 1} \left|C_n^{\lambda}(x)\right| = \binom{n+2\lambda-1}{n}$$

and for $\alpha = \beta = 0$

$$\max_{-1\le x\le 1} |P_n(x)| = 1.$$

Theorem 1.2.11 *For every α, $\beta > -1$ and $n \in \mathbb{N}_0$, the norm of $P_n^{(\alpha,\beta)}$ is given by*

$$\left\|P_n^{(\alpha,\beta)}\right\|^2_{\mathrm{L}^2_w[-1,1]} = \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1} \cdot \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{n!\,\Gamma(n+\alpha+\beta+1)}. \tag{1.39}$$

We can also determine the norm for the Gegenbauer polynomials, i.e. for $\alpha = \beta = \lambda - \frac{1}{2}$, (1.39) yields

$$\begin{aligned}
\left\|C_n^{\lambda}\right\|^2_{\mathrm{L}^2_w[-1,1]} &= \left\|\frac{\Gamma(\lambda+\frac{1}{2})\Gamma(n+2\lambda)}{\Gamma(2\lambda)\Gamma(n+\lambda+\frac{1}{2})} P_n^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}\right\|^2_{\mathrm{L}^2_w[-1,1]} \\
&= \left(\frac{\Gamma(\lambda+\frac{1}{2})\Gamma(n+2\lambda)}{\Gamma(2\lambda)\Gamma(n+\lambda+\frac{1}{2})}\right)^2 \left\|P_n^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}\right\|^2_{\mathrm{L}^2_w[-1,1]} \\
&= \left(\frac{\Gamma(\lambda+\frac{1}{2})\Gamma(n+2\lambda)}{\Gamma(2\lambda)\Gamma(n+\lambda+\frac{1}{2})}\right)^2 \frac{2^{2\lambda}\left(\Gamma(n+\lambda+\frac{1}{2})\right)^2}{(2n+2\lambda)\Gamma(n+1)\Gamma(n+2\lambda)} \\
&= \frac{2^{2\lambda}}{2n+2\lambda} \frac{\Gamma(n+2\lambda)}{\Gamma(n+1)} \left(\frac{\Gamma(\lambda+\frac{1}{2})}{\Gamma(2\lambda)}\right)^2.
\end{aligned}$$

Using the duplication formula (see Lemma 1.1.4) for $x = 2\lambda$, we get

$$\left\|C_n^{\lambda}\right\|^2_{\mathrm{L}^2_w[-1,1]} = \frac{\Gamma(n+2\lambda)}{(n+\lambda)n!} 2^{2\lambda-1} \left(\frac{\sqrt{\pi}}{2^{2\lambda-1}\Gamma(\lambda)}\right)^2.$$

Further simplification yields the norm of C_n^{λ} as

$$\left\|C_n^{\lambda}\right\|^2_{\mathrm{L}^2_w[-1,1]} = \frac{\Gamma(n+2\lambda)}{(n+\lambda)n!} \frac{2^{1-2\lambda}}{\left(\Gamma(\lambda)\right)^2}\pi. \tag{1.40}$$

Also, for $\alpha = \beta = 0$, (1.39) reduces to the norm of Legendre polynomials P_n, i.e.

$$\|P_n\|^2_{\mathrm{L}^2[-1,1]} = \frac{2}{2n+1}. \tag{1.41}$$

1.3 Spherical Harmonics

This section briefly introduces spherical harmonics and some of their notable results (see for details [19, 53]). These functions, defined on the surface of a ball, are well known in the field of geosciences.

Definition 1.3.1 *Let $D \subset \mathbb{R}^3$ be open and connected. A function $F \in \mathrm{C}^2(D)$ is called harmonic if and only if*

$$\Delta_x F(x) = 0 \text{ for all } x \in D.$$

The set of all harmonic functions in $\mathrm{C}^2(D)$ is denoted by $\mathrm{Harm}(D)$.

Definition 1.3.2 *A polynomial P in $\mathbb{R}^3$ is called a homogeneous polynomial of degree n, if*

$$P(\lambda x) = \lambda^n P(x)$$

for all $\lambda \in \mathbb{R}$ and $x \in \mathbb{R}^3$. $\mathrm{Hom}_n(\mathbb{R}^3)$ denotes the class of all homogeneous polynomials of degree n.

Theorem 1.3.3 *For $n \in \mathbb{N}_0$, the dimension of $\mathrm{Hom}_n(\mathbb{R}^3)$ is given as*

$$\dim\left(\mathrm{Hom}_n(\mathbb{R}^3)\right) = \frac{(n+1)(n+2)}{2}.$$

Definition 1.3.4 *The set of all homogeneous harmonic polynomials on $\mathbb{R}^3$ with degree $n \in \mathbb{N}_0$ is denoted by $\mathrm{Harm}_n(\mathbb{R}^3)$, i.e.*

$$\mathrm{Harm}_n(\mathbb{R}^3) := \{P \in \mathrm{Hom}_n(\mathbb{R}^3) \mid \Delta P = 0\}, \quad n \in \mathbb{N}_0.$$

Definition 1.3.5 *Spherical harmonics Y_n are the restrictions of the polynomials $P_n \in \mathrm{Harm}_n(\mathbb{R}^3)$ to the sphere Ω, i.e.*

$$\mathrm{Harm}_n(\Omega) := \{Y_n : Y_n = P_n|_\Omega, P_n \in \mathrm{Harm}_n(\mathbb{R}^3)\}.$$

Definition 1.3.6 *For degree n and order j, the spherical harmonic $Y_{n,j}$ denotes a member of an orthonormal system $\{Y_{n,j} \mid n \in \mathbb{N}_0, j = 1, 2, \ldots, 2n+1\}$ with respect to $\langle \cdot, \cdot \rangle_{\mathrm{L}^2(\Omega)}$.*

Theorem 1.3.7 *The space $\mathrm{Harm}_n(\Omega)$ and its elements Y_n have the following properties:*

1. *The dimension of the space $\mathrm{Harm}_n(\Omega)$ is given as*

$$\dim(\mathrm{Harm}_n(\Omega)) = 2n + 1, \quad n \in \mathbb{N}_0.$$

2. *Y_n is an eigenfunction of the Beltrami operator Δ^* corresponding to the eigenvalues $-n(n+1)$, i.e.*

$$\Delta^*_\xi Y_n(\xi) = -n(n+1)Y_n(\xi), \quad n \in \mathbb{N}_0,\ \xi \in \Omega. \tag{1.42}$$

3. *For every $Y_n \in \mathrm{Harm}_n(\Omega)$, $Y_m \in \mathrm{Harm}_m(\Omega)$ and $n, m \in \mathbb{N}_0$*

$$\langle Y_n, Y_m \rangle_{\mathrm{L}^2(\Omega)} = 0, \quad \text{if } n \neq m.$$

4. *For every $Y_n \in \mathrm{Harm}_n(\Omega)$,*

$$\|Y_n\|_{\mathrm{C}(\Omega)} \leq \sqrt{\frac{2n+1}{4\pi}} \|Y_n\|_{\mathrm{L}^2(\Omega)}, \quad n \in \mathbb{N}_0. \tag{1.43}$$

In particular,

$$\|Y_{n,j}\|_{\mathrm{C}(\Omega)} \leq \sqrt{\frac{2n+1}{4\pi}}. \tag{1.44}$$

Theorem 1.3.8 *The operator $\left(-\Delta^* + \frac{1}{4}\right) : \mathrm{C}^2(\Omega) \to \mathrm{C}(\Omega)$ is an injective differentiable operator with $Y_{n,j}$ as eigenfunctions corresponding to the eigenvalues ([24])*

$$\left(-\Delta^* + \frac{1}{4}\right)^\wedge (n) = \left(n + \frac{1}{2}\right)^2, \quad n \in \mathbb{N}_0. \tag{1.45}$$

Theorem 1.3.9 *For $n \in \mathbb{N}_0$ and $j \in \{1, 2, \ldots, 2n+1\}$, the system $\{Y_{n,j}\}$ fulfils the following attributes:*

1. *For all $j, k \in \{1, 2, \ldots, 2n+1\}$ and $n, m \in \mathbb{N}_0$*

$$\langle Y_{n,j}, Y_{m,k} \rangle_{\mathrm{L}^2(\Omega)} = \delta_{nm}\delta_{jk}. \tag{1.46}$$

2. *For $F \in \mathrm{Harm}_n(\Omega)$ and for all $j \in \{1, 2, \ldots, 2n+1\}$*

$$\langle F, Y_{n,j} \rangle_{\mathrm{L}^2(\Omega)} = 0 \implies F = 0.$$

Hence, for each $n \in \mathbb{N}_0$, $\{Y_{n,j}\}_{j=1,2,\ldots,2n+1}$ forms a complete orthonormal basis for $\mathrm{Harm}_n(\Omega)$. In addition, $\{Y_{n,j}\}_{n\in\mathbb{N}_0; j=1,2,\ldots,2n+1}$ forms a complete orthonormal system in the Hilbert space $(\mathrm{L}^2(\Omega), \langle\cdot,\cdot\rangle_{\mathrm{L}^2(\Omega)})$.

By virtue of the above result, every $F \in \mathrm{L}^2(\Omega)$ can be expanded in a Fourier series, i.e.

$$F = \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} F^\wedge(n,j) Y_{n,j} \tag{1.47}$$

converges in the $\mathrm{L}^2(\Omega)$-sense, where $F^\wedge(n,j) = \langle F, Y_{n,j} \rangle_{\mathrm{L}^2(\Omega)}$ are the Fourier coefficients.

Theorem 1.3.10 (Parseval Identity). *For every F, $G \in \mathrm{L}^2(\Omega)$, the Parseval identity holds, i.e.*

$$\langle F, G\rangle_{\mathrm{L}^2(\Omega)} = \sum_{n=0}^{\infty}\sum_{j=1}^{2n+1} \langle F, Y_{n,j}\rangle_{\mathrm{L}^2(\Omega)} \langle G, Y_{n,j}\rangle_{\mathrm{L}^2(\Omega)} . \tag{1.48}$$

Theorem 1.3.11 (Addition Theorem for Spherical Harmonics). *Let $\{Y_{n,j}\}_{n\in\mathbb{N}_0;j=1,2,\ldots,2n+1}$ be as defined above and P_n be the Legendre polynomial of degree n, then*

$$\sum_{j=1}^{2n+1} Y_{n,j}(\xi)Y_{n,j}(\eta) = \frac{2n+1}{4\pi}P_n(\xi\cdot\eta), \quad \xi,\eta\in\Omega. \tag{1.49}$$

1.4 Orthonormal Systems on the Ball

At present, inverse problems and approximation methods have important applications in various fields. In particular, these methods play a vital role in the field of geosciences. Primarily, an approach for inverse problems and likewise for constructive approximation is the expansion of the solution in an orthonormal basis and mostly orthogonal polynomials are favourable as such basis. For example, Legendre polynomials serve as an orthogonal basis system on $[-1,1]$ and spherical harmonics establish an orthonormal basis for the sphere. Likewise two such systems, denoted by $G^{\mathrm{X}}_{m,n,j}$ for $\mathrm{X}\in\{\mathrm{I},\mathrm{II}\}$, are constructed on the 3-dimensional ball $\mathcal{B}_R$ (see [4, 26, 45, 46, 47, 72]). These systems are denoted and defined as follows.

Theorem 1.4.1 *For $m,n\in\mathbb{N}_0$; $j\in\{1,2,\ldots,2n+1\}$, the systems of functions $G^{\mathrm{I}}_{m,n,j}$ and $G^{\mathrm{II}}_{m,n,j}$ defined on $\mathcal{B}_R$ as*

$$G^{\mathrm{I}}_{m,n,j}(x) := \sqrt{\frac{4m+2l_n+3}{R^3}}P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{|x|^2}{R^2}-1\right)\left(\frac{|x|}{R}\right)^{l_n} Y_{n,j}\left(\frac{x}{|x|}\right), \quad x\in\mathcal{B}_R\setminus\{0\}, \tag{1.50}$$

where $l_n \geq -1$ and

$$G^{\mathrm{II}}_{m,n,j}(x) := \sqrt{\frac{2m+3}{R^3}}P_m^{(0,2)}\left(2\frac{|x|}{R}-1\right)Y_{n,j}\left(\frac{x}{|x|}\right), \ x\in\mathcal{B}_R\setminus\{0\}, \tag{1.51}$$

form orthonormal systems in $\mathrm{L}^2(\mathcal{B}_R)$.

These basis systems are comprised of spherical harmonics (angular part) and Jacobi polynomials (radial part) and differ in the choice of the radial part. The exponent l_n in the type I system depends on n for all $n \in \mathbb{N}_0$. Two particular cases for this exponent are known, that are: $l_n = n$, that relates to the inverse gravimetric problem and $l_n = n-1$, that corresponds to the inverse magnetic problem (see, for example [61, 68] for a description of these problems). Some of the properties of these systems are investigated, for example, in [2, 47, 50].

Theorem 1.4.2 *The orthonormal basis system of type* I *has the following properties:*

1. *For $n \in \mathbb{N}_0$; $j \in \{1, 2, \dots, 2n+1\}$, $G^{\mathrm{I}}_{m,n,j}$ is harmonic if and only if $m = 0$ and $l_n = n$ or $l_0 = -1$.*

2. *For $m, n \in \mathbb{N}_0$; $j \in \{1, 2, \dots, 2n+1\}$ and $l_n = n$, $G^{\mathrm{I}}_{m,n,j}$ is an algebraic polynomial with degree $2m+n$.*

Proof:

1. It is clear that for $m = 0$ and $l_n = n \in \mathbb{N}_0$ or $l_0 = -1$, $G^{\mathrm{I}}_{m,n,j}$ is harmonic. Conversely, we assume that $G^{\mathrm{I}}_{m,n,j}$ is harmonic, then

$$\Delta_{r\xi}\left(G^{\mathrm{I}}_{m,n,j}(r\xi)\right) = 0$$
$$\Delta_{r\xi}\left(F_m(r) Y_{n,j}(\xi)\right) = 0,$$

where $F_m(r) = \left(\frac{r}{R}\right)^{l_n} P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{r^2}{R^2} - 1\right)$. Using the Laplace operator (1.3), we have

$$\left(F''_m(r) + \frac{2}{r}F'_m(r) - \frac{n(n+1)}{r^2}F_m(r)\right) Y_{n,j}(\xi) = 0 \text{ for all } r > 0,\ \xi \in \Omega$$
$$\Leftrightarrow F''_m(r) + \frac{2}{r}F'_m(r) - \frac{n(n+1)}{r^2}F_m(r) = 0 \text{ for all } r > 0$$
$$\Leftrightarrow r^2 F''_m(r) + 2rF'_m(r) - n(n+1)F_m(r) = 0 \text{ for all } r > 0.$$

Here, we have a second order ordinary differential equation having solutions

$$F_m(r) = \text{const} \cdot r^n \quad \text{and } F_m(r) = \text{const} \cdot r^{-n-1}.$$

For $F_m(r) = \text{const} \cdot r^n$, we have

$$\left(\frac{r}{R}\right)^{l_n} P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{r^2}{R^2} - 1\right) = \text{const} \cdot r^n$$
$$\Leftrightarrow \left(\frac{1}{R}\right)^{l_n} P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{r^2}{R^2} - 1\right) = \text{const} \cdot r^{n-l_n}.$$

By the use of equation (1.34) for $\beta = l_n + \frac{1}{2}$, the above equation yields

$$\left(\frac{1}{R}\right)^{l_n} \sum_{k=0}^{m} (-1)^{m-k} \binom{m}{k} \binom{l_n + \frac{1}{2} + k + m}{m} \left(\frac{r}{R}\right)^{2k} = \text{const} \cdot r^{n-l_n}.$$

Since on the right hand side we have a monomial, the above equality exists only if $m = 0$, which implies $n = l_n$. Similar calculations can be done for the other solution which gives $l_n = -(n+1)$. Due to our restriction on l_n, i.e. $l_n \geq -1$, this solution is only possible if $n = 0$.

2. We already know that $\left(\frac{r}{R}\right)^n Y_{n,j}(\xi)$ is a polynomial with degree n and $P_m^{(0,n+\frac{1}{2})}\left(2\frac{r^2}{R^2} - 1\right)$ is a polynomial with degree $2m$. Hence, for $m, n \in \mathbb{N}_0$ and $l_n = n$, the construction of $G^{\mathrm{I}}_{m,n,j}$ allows us to state that it is an algebraic polynomial with degree $2m + n$.

■

Theorem 1.4.3 *For $m, n \in \mathbb{N}_0$, $l_n \geq 0$; $j \in \{1, 2, \ldots, 2n+1\}$, an upper bound for the maximum norm of the basis systems* (1.50) *and* (1.51) *respectively, is given by*

$$\left\| G^{\mathrm{I}}_{m,n,j} \right\|_{\mathrm{C}(\mathcal{B}_R)} \leq \sqrt{\frac{(4m + 2l_n + 3)(2n+1)}{4\pi R^3}} \binom{m + l_n + \frac{1}{2}}{m} \tag{1.52}$$

and

$$\left\| G^{\mathrm{II}}_{m,n,j} \right\|_{\mathrm{C}(\mathcal{B}_R)} \leq \sqrt{\frac{(2m+3)(2n+1)}{4\pi R^3}} \frac{(m+2)(m+1)}{2}. \tag{1.53}$$

Proof: From Theorem 1.2.10 for Jacobi polynomials, we know that

$$\max_{-1 \leq x \leq 1} \left| P_m^{(\alpha,\beta)}(x) \right| = \binom{m+q}{m},$$

where $q = \max(\alpha, \beta)$. For system II, it is clear that $q = 2$, which implies

$$\max_{-1 \leq x \leq 1} \left| P_m^{(0,2)}\left(2\frac{|x|}{R} - 1\right) \right| = \frac{(m+2)(m+1)}{2}.$$

The above equation together with the maximum norm of spherical harmonics (1.44) gives us the required inequality (1.53).
The system of type I (1.50) depends on the term l_n, where $l_n \geq -1$. Since

the term $\left(\frac{|x|}{R}\right)^{l_n} \geq 1$ for negative values of l_n, we restrict l_n only to positive values, i.e. $l_n \geq 0$. This implies $l_n + \frac{1}{2} > 0$ and, as a consequence, we obtain

$$\max_{-1\leq x\leq 1} \left| P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{|x|^2}{R^2} - 1\right)\right| = \binom{m + l_n + \frac{1}{2}}{m}, \quad l_n > -\frac{1}{2}. \tag{1.54}$$

Further, $\left(\frac{|x|}{R}\right)^{l_n} \leq 1$ for $l_n \geq 0$. This gives us the desired result (1.52) and completes the proof. ■

The composition of two (particular) invertible differential operators results in an invertible differential operator for the systems (1.50) and (1.51) (for details and proofs, see [2, 50]).

Theorem 1.4.4 *For $m, n \in \mathbb{N}_0$; $j \in \{1, 2, \dots, 2n+1\}$, $G^{\mathrm{I}}_{m,n,j}$ forms an eigenfunction of the invertible differential operator*

$$\Delta^{\mathrm{I}}_x = \left(-D^{\mathrm{I}}_{|x|} + \frac{9}{4}\right) \circ \left(-\Delta^*_{\frac{x}{|x|}} + \frac{1}{4}\right), \tag{1.55}$$

corresponding to the eigenvalues $\left(\frac{(4m+2l_n+3)(2n+1)}{4}\right)^2$ *and* $G^{\mathrm{II}}_{m,n,j}$ *is an eigenfunction of*

$$\Delta^{\mathrm{II}}_x = \left(-D^{\mathrm{II}}_{|x|} + \frac{9}{4}\right) \circ \left(-\Delta^*_{\frac{x}{|x|}} + \frac{1}{4}\right), \tag{1.56}$$

corresponding to the eigenvalues $\left(\frac{(2m+3)(2n+1)}{4}\right)^2$.

In the above result, Δ^* denotes the Beltrami operator from Equation (1.42) and D^{X}_r, for $r := |x|$, represents a differential operator given as

$$D^{\mathrm{X}}_r = \begin{cases} (R^2 - r^2)\frac{\mathrm{d}^2}{\mathrm{d}r^2} + 2\left(1 - 2\frac{r^2}{R^2}\right)\frac{R^2}{r}\frac{\mathrm{d}}{\mathrm{d}r} - n(n+1)\frac{R^2}{r^2}, & \mathrm{X} = \mathrm{I}, \\ rR\left(1 - \frac{r}{R}\right)\frac{\mathrm{d}^2}{\mathrm{d}r^2} + (3R - 4r)\frac{\mathrm{d}}{\mathrm{d}r}, & \mathrm{X} = \mathrm{II}. \end{cases} \tag{1.57}$$

Now based on the basis systems (1.50) and (1.51), we give the concept of Sobolev spaces on $\mathcal{B}_R$, which follows from [26, 46, 47].

Definition 1.4.5 *For* $\mathrm{X} \in \{\mathrm{I}, \mathrm{II}\}$*, a Sobolev space on* $\mathcal{B}_R$ *depending on a sequence* $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ *and an orthonormal system* $\{G^{\mathrm{X}}_{m,n,j}\}_{m,n\in\mathbb{N}_0;\, j=1,\dots,2n+1}$ *is the space*

$$\mathcal{H}(\mathcal{B}_R) := \mathcal{H}(\{A_{m,n}\}, \mathrm{X}, \mathcal{B}_R)$$

containing all functions $F \in \mathrm{L}^2(\mathcal{B}_R)$ *such that*

$$\left\langle F, G^{\mathrm{X}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} = 0$$

for all (m,n,j) *with* $A_{m,n}=0$ *or* $l_n<0$ *and*

$$\sum_{m,n=0}^{\infty}\sum_{j=1}^{2n+1} A_{m,n}^2 \left\langle F, G_{m,n,j}^{\mathrm{X}}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)}^2 < +\infty.$$

The inner product in $\mathcal{H}$ *is defined as*

$$\langle F_1,F_2\rangle_{\mathcal{H}} := \sum_{m,n=0}^{\infty}\sum_{j=1}^{2n+1} A_{m,n}^2 \left\langle F_1, G_{m,n,j}^{\mathrm{X}}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} \left\langle F_2, G_{m,n,j}^{\mathrm{X}}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)}.$$

For further results, we simplify the following double summation for a sequence $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$:

$$\sum_{\substack{m,n=0\\A_{m,n}\neq 0}}^{\infty}\sum_{j=1}^{2n+1} A_{m,n}^{-2}\left(G_{m,n,j}^{\mathrm{X}}(x)\right)^2 = \sum_{\substack{m,n=0\\A_{m,n}\neq 0}}^{\infty}\sum_{j=1}^{2n+1} A_{m,n}^{-2}\left(F_{m,n}^{\mathrm{X}}(|x|)Y_{n,j}\left(\frac{x}{|x|}\right)\right)^2, \tag{1.58}$$

where

$$F_{m,n}^{\mathrm{X}}(|x|) := \begin{cases} \sqrt{\frac{4m+2l_n+3}{R^3}}P_m^{(0,l_n+\frac12)}\left(2\frac{|x|^2}{R^2}-1\right)\left(\frac{|x|}{R}\right)^{l_n}, & \mathrm{X}=\mathrm{I},\\ \sqrt{\frac{2m+3}{R^3}}P_m^{(0,2)}\left(2\frac{|x|}{R}-1\right), & \mathrm{X}=\mathrm{II}.\end{cases} \tag{1.59}$$

By means of the addition theorem 1.3.11, (1.58) takes the subsequent form

$$\sum_{\substack{m,n=0\\A_{m,n}\neq 0}}^{\infty}\sum_{j=1}^{2n+1} A_{m,n}^{-2}\left(F_{m,n}^{\mathrm{X}}(|x|)Y_{n,j}\left(\frac{x}{|x|}\right)\right)^2 = \sum_{\substack{m,n=0\\A_{m,n}\neq 0}}^{\infty} A_{m,n}^{-2}\frac{2n+1}{4\pi}\left(F_{m,n}^{\mathrm{X}}(|x|)\right)^2.$$

Due to the same reasoning in Theorem 1.4.3, we have to restrict again the values of l_n to positive real numbers so that

$$\left(\frac{|x|}{R}\right)^{l_n}\le 1.$$

Hence, using Theorem 1.2.10, we have

$$\sum_{\substack{m,n=0\\A_{m,n}\neq 0}}^{\infty}\sum_{j=1}^{2n+1} A_{m,n}^{-2}\left(F_{m,n}^{\mathrm{X}}(|x|)Y_{n,j}\left(\frac{x}{|x|}\right)\right)^2$$
$$\le \begin{cases}\sum\limits_{\substack{m,n=0\\A_{m,n}\neq 0}}^{\infty} A_{m,n}^{-2}\frac{(4m+2l_n+3)(2n+1)}{4\pi R^3}\binom{m+l_n+\frac12}{m}^2, & \mathrm{X}=\mathrm{I},\\ \sum\limits_{\substack{m,n=0\\A_{m,n}\neq 0}}^{\infty} A_{m,n}^{-2}\frac{(2m+3)(2n+1)}{4\pi R^3}\binom{m+2}{m}^2, & \mathrm{X}=\mathrm{II}.\end{cases}$$

For the case of type I, the above inequality can be simplified further as follows: For $l_n > -\frac{1}{2}$,

$$\begin{aligned} \binom{m+l_n+\frac{1}{2}}{m} &= \frac{\Gamma(m+l_n+\frac{3}{2})}{\Gamma(m+1)\Gamma(l_n+\frac{3}{2})} \\ &= \frac{\Gamma(l_n+\frac{3}{2})}{\Gamma(m+1)\Gamma(l_n+\frac{3}{2})} \prod_{k=\frac{3}{2}}^{m+\frac{1}{2}} (l_n+k) \\ &= \frac{1}{\Gamma(m+1)} \prod_{k=\frac{3}{2}}^{m+\frac{1}{2}} (l_n+k), \\ \binom{m+l_n+\frac{1}{2}}{m} &\leq \frac{(l_n+m+\frac{1}{2})^m}{m!}. \end{aligned} \tag{1.60}$$

Similarly, for type II, we have

$$\begin{aligned} \binom{m+2}{m} &= \frac{\Gamma(m+3)}{\Gamma(m+1)\Gamma(3)} \\ &= \frac{(m+2)(m+1)}{2} \\ &\leq \frac{(2m+3)(2m+3)}{2}, \\ \binom{m+2}{m} &\leq \frac{(2m+3)^2}{2}. \end{aligned} \tag{1.61}$$

Hence, we get the refined form of (1.58) as

$$\sum_{\substack{m,n=0 \\ A_{m,n}\neq 0}}^{\infty} \sum_{j=1}^{2n+1} A_{m,n}^{-2} \left(G_{m,n,j}^{\mathrm{X}}(x)\right)^2$$
$$\leq \begin{cases} \sum\limits_{\substack{m,n=0 \\ A_{m,n}\neq 0}}^{\infty} A_{m,n}^{-2} \frac{(4m+2l_n+3)(2n+1)}{4\pi R^3} \frac{(l_n+m+\frac{1}{2})^{2m}}{(m!)^2}, & \mathrm{X} = \mathrm{I}, \\ \sum\limits_{\substack{m,n=0 \\ A_{m,n}\neq 0}}^{\infty} A_{m,n}^{-2} \frac{(2m+3)^5(2n+1)}{16\pi R^3}, & \mathrm{X} = \mathrm{II}. \end{cases} \tag{1.62}$$

We now define a condition on the sequence $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$, that promises the continuity of the function $F \in \mathcal{H}(\mathcal{B}_R)$ with a uniformly convergent Fourier series on $\mathcal{B}_R$.

Definition 1.4.6 (Summability Condition). *A sequence* $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ *is said to satisfy the summability condition of type* I *if*

$$\sum_{\substack{m,n=0;\, l_n\geq -\frac{1}{2}\\ A_{m,n}\neq 0}}^{\infty} A_{m,n}^{-2}\,(2n+1)(4m+2l_n+3)\frac{(l_n+m+\frac{1}{2})^{2m}}{(m!\,)^2} < +\infty, \tag{1.63}$$

and the summability condition of type II *is given as*

$$\sum_{\substack{m,n=0\\ A_{m,n}\neq 0}}^{\infty} A_{m,n}^{-2}\,(2n+1)(2m+3)^5 < +\infty. \tag{1.64}$$

If a sequence fulfils the summability condition of type I *or* II*, we say that the sequence is* I- *or* II-summable*, respectively.*

The summability condition allows us to state the following result.

Lemma 1.4.7 (Sobolev Lemma). *Let* $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ *be a summable sequence, then for every* $F\in\mathcal{H}(\mathcal{B}_R)$*, the Fourier series*

$$F(x) = \sum_{m,n=0}^{\infty}\sum_{j=1}^{2n+1}\left\langle F, G^{\mathrm{X}}_{m,nj}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} G^{\mathrm{X}}_{m,n,j}(x), \quad \mathrm{X}\in\{\mathrm{I},\mathrm{II}\}, \tag{1.65}$$

is uniformly convergent on $\mathcal{B}_R$*. Also, every function* $F\in\mathcal{H}(\mathcal{B}_R)$ *is continuous on* $\mathcal{B}_R\setminus\{0\}$*.*

Proof: In order to prove the uniform convergence of (1.65), we consider

$$\begin{aligned}&\left|\sum_{m=M}^{\infty}\sum_{n=N}^{\infty}\sum_{j=1}^{2n+1}\left\langle F, G^{\mathrm{X}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} G^{\mathrm{X}}_{m,n,j}(x)\right|\\ &= \left|\sum_{\substack{m=M\\ A_{m,n}\neq 0}}^{\infty}\sum_{n=N}^{\infty}\sum_{j=1}^{2n+1} A_{m,n}\left\langle F, G^{\mathrm{X}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} A_{m,n}^{-1} G^{\mathrm{X}}_{m,n,j}(x)\right|.\end{aligned}$$

Using the Cauchy-Schwarz Inequality (1.17), we get

$$\left|\sum_{m=M}^{\infty}\sum_{n=N}^{\infty}\sum_{j=1}^{2n+1}\left\langle F, G^{\mathrm{X}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} G^{\mathrm{X}}_{m,n,j}(x)\right|$$

$$\leq \left(\sum_{m=M}^{\infty}\sum_{n=N}^{\infty}\sum_{j=1}^{2n+1} A^2_{m,n}\left\langle F, G^{\mathrm{X}}_{m,n,j}\right\rangle^2_{\mathrm{L}^2(\mathcal{B}_R)}\right)^{\frac{1}{2}}\left(\sum_{\substack{m=M\\A_{m,n}\neq 0}}^{\infty}\sum_{n=N}^{\infty}\sum_{j=1}^{2n+1} A^{-2}_{m,n}\left(G^{\mathrm{X}}_{m,n,j}(x)\right)^2\right)^{\frac{1}{2}}$$

$$\leq \|F\|_{\mathcal{H}(\mathcal{B}_R)}\left(\sum_{\substack{m=M\\A_{m,n}\neq 0}}^{\infty}\sum_{n=N}^{\infty}\sum_{j=1}^{2n+1} A^{-2}_{m,n}\left(G^{\mathrm{X}}_{m,n,j}(x)\right)^2\right)^{\frac{1}{2}}.$$

Due to the summability conditions (1.63) and (1.64), the second term on the right hand side of the inequality is finite and converges to zero for $M, N \to \infty$. This implies the convergence of the series in (1.65). Further, as $G^{\mathrm{X}}_{m,n,j}$ is continuous on $\mathcal{B}_R\backslash\{0\}$ and (1.65) converges uniformly, so from the uniform convergence theorem 1.1.26, F is continuous on $\mathcal{B}_R\backslash\{0\}$. ■

Remark 1.4.8 *For the particular case* $\mathrm{X} = \mathrm{I}$ *with* $l_n = n$, F *is also continuous on* $\mathcal{B}_R$.

It is also clear from the above result, that the evaluation functional $\mathcal{L}_x$

$$\begin{aligned}\mathcal{L}_x : \mathcal{H} &\to \mathbb{R}\\ F &\mapsto F(x)\end{aligned}$$

for every fixed $x \in \mathcal{B}_R$, is bounded and hence continuous. Thus, from Aronszajn's theorem 1.1.16, the Sobolev space $\mathcal{H}$ on $\mathcal{B}_R$ is a reproducing kernel Hilbert space equipped with the kernel $K_{\mathcal{H}}$ (see [46], Theorem 25) defined as

$$K_{\mathcal{H}}(x,y) = \sum_{\substack{m=0\\A_{m,n}\neq 0,\, l_n\geq 0}}^{\infty}\sum_{n=0}^{\infty}\sum_{j=1}^{2n+1} A^{-2}_{m,n} G^{\mathrm{X}}_{m,n,j}(x) G^{\mathrm{X}}_{m,n,j}(y), \quad x, y \in \mathcal{B}_R. \tag{1.66}$$

Theorem 1.4.9 *Let* $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ *be a summable sequence, then* $\mathcal{H}$ *has a unique reproducing kernel defined by* (1.66).

1.5 Statistical Preliminaries

In this section, we give some basic definitions, results and properties from stochastics and statistics which are used in our work (for details, see [16, 67, 69, 74]).
A function that assigns a random numerical (real) value to every outcome of an experiment is known as a random variable. We state here some of the properties of random variables.

Definition 1.5.1 *The function f is a probability density function (pdf) for the continuous random variable X, defined over $\mathbb{R}$, if*

1. $f(x) \geq 0$ *for all* $x \in \mathbb{R}$.
2. $\int_{-\infty}^{\infty} f(x)\,\mathrm{d}x = 1$.
3. $\mathbb{P}(a < X < b) = \int_a^b f(x)\,\mathrm{d}x$.

Definition 1.5.2 *The distribution function F_X of a random variable X with density function f is the probability that X will be less or equal to a given value $x \in \mathbb{R}$, i.e.*

$$F_X(x) = \mathbb{P}(X \leq x).$$

Definition 1.5.3 *A collection of random variables is known as independent and identically distributed (i.i.d.) random variables, if each variable has the same probability distribution and the variables are independent of each other.*

Definition 1.5.4 *For a continuous random variable X, the expectation of $g(X)$ on a measurable space $\mathcal{V}$ along with a probability measure $\mathcal{P}$ is defined as*

$$\mathbb{E}[g(X)] = \int_{\mathcal{V}} g(X)\mathrm{d}\mathcal{P}(X). \tag{1.67}$$

The probability measure $\mathcal{P}$ is given by

$$\mathcal{P}(A) := \int_A f(x)\mathrm{d}\mu(x), \quad A \in \mathcal{V},$$

where $f = \frac{\mathrm{d}\mathcal{P}}{\mathrm{d}\mu}$ is the density of $\mathcal{P}$ with respect to the measure μ of space $\mathcal{V}$. Hence, in terms of the density function f, the expectation of $g(X)$ is given by

$$\mathbb{E}[g(X)] = \int_{infty}^{\infty} g(x)f(x)\mathrm{d}\mu(x) \tag{1.68}$$

and the variance of $g(X)$ is

$$\begin{aligned} \mathbb{V}[g(X)] &= \mathbb{E}\left[(g(X) - \mathbb{E}(g(X)))^2\right] \\ &= \mathbb{E}[g(X)]^2 - (\mathbb{E}[g(X)])^2 . \end{aligned} \tag{1.69}$$

We state below some basic and important properties for expectation and variance of random variables.

Theorem 1.5.5 *Let X and Y be any random variables.*

- *If X and Y are independent, then $g(X)$ and $h(Y)$ are also independent for any functions g and h. Also*

$$\mathbb{E}(XY) = \mathbb{E}(X)\mathbb{E}(Y). \tag{1.70}$$

More generally, the following holds for any functions g and h:

$$\mathbb{E}(g(X)h(Y)) = \mathbb{E}(g(X))\mathbb{E}(h(Y)). \tag{1.71}$$

- *For any constants a and b,*

$$\mathbb{E}(aX + b) = a\mathbb{E}(X) + b \tag{1.72}$$

and since $\mathbb{V}(b) = 0$, we have

$$\mathbb{V}(aX + b) = a^2\mathbb{V}(X). \tag{1.73}$$

- *In general, for any finite collection of random variables $X_1, X_2, \ldots, X_n$ with finite expectations, the following holds:*

$$\mathbb{E}\left[\sum_{k=1}^{n} X_k\right] = \sum_{k=1}^{n} \mathbb{E}[X_k]. \tag{1.74}$$

This property is known as the linearity of expectation ([52]), i.e. the expectation of the sum of random variables is equal to the sum of their expectations. Also, linearity of expectations holds for countably infinite summations, i.e.

$$\mathbb{E}\left[\sum_{k=1}^{\infty} X_k\right] = \sum_{k=1}^{\infty} \mathbb{E}[X_k], \tag{1.75}$$

whenever $\sum_{k=1}^{\infty} \mathbb{E}[X_k]$ converges.

- *Monotonicity of expectation: If $X \leq Y$, then the inequality*

$$\mathbb{E}(X) \leq \mathbb{E}(Y) \tag{1.76}$$

holds, given the expectations exist. Additionally, if $|X| \leq C$, C being constant, then $\mathbb{E}|X| \leq C$.

- *Cauchy-Schwarz inequality for expectation: For any random variables X and Y, we have*

$$\mathbb{E}|XY| \leq \sqrt{\mathbb{E}(X^2)}\sqrt{\mathbb{E}(Y^2)}. \tag{1.77}$$

- *Minkowski's inequality for expectation: Let $\{X_k\}_{k\geq 1}$ be a collection of random variables. If $p \geq 1$, then*

$$\left[\mathbb{E}\left|\sum_{k=1}^{\infty} X_k\right|^p\right]^{\frac{1}{p}} \leq \sum_{k=1}^{\infty} \left[\mathbb{E}\,|X_k|^p\right]^{\frac{1}{p}}. \tag{1.78}$$

Theorem 1.5.6 *If $\{X_k\}_{k\geq 1}$ is a collection of independent random variables with finite expectations, then*

$$\mathbb{V}\left[\sum_{k=1}^{\infty} X_k\right] = \sum_{k=1}^{\infty} \mathbb{V}[X_k]. \tag{1.79}$$

A specific and widely used type of random variables is known as the normal random variable.

Definition 1.5.7 *For any real numbers μ and $\sigma > 0$, the Gaussian or normal probability density function with mean μ and variance σ^2 is defined by*

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}.$$

A random variable X having the density function f is said to be a normally distributed random variable $X \sim \mathcal{N}(\mu, \sigma^2)$ with μ and σ^2 being the mean and variance, respectively.

Definition 1.5.8 *A normal random variable X with expectation 0 and variance 1 is named as a standard normal random variable. The sum of n squared standard normal variables is a χ^2-random variable with n degrees of freedom, i.e.*

$$\chi^2(n) = \sum_{k=1}^{n} X_k^2.$$

Definition 1.5.9 *For a random variable X, the function $\phi_X : \mathbb{R} \to \mathbb{C}$ defined by*

$$\phi_X(t) = \mathbb{E}\left(e^{itX}\right), \quad t \in \mathbb{R},$$

is called a characteristic function of X. Here, i denotes the complex number with $i^2 = -1$.

Theorem 1.5.10 *For independent random variables X_1 and X_2, the characteristic function of $X_1 + X_2$ is given by*

$$\phi_{X_1+X_2} = \phi_{X_1}\phi_{X_2}.$$

Theorem 1.5.11 *The expectation, variance and characteristic function of a χ^2-random variable with n degrees of freedom, respectively are*

$$\mathbb{E}\left(\chi^2(n)\right) = n, \tag{1.80}$$

$$\mathbb{V}\left(\chi^2(n)\right) = 2n, \tag{1.81}$$

$$\phi_{\chi^2(n)}(t) = (1-2it)^{-\frac{n}{2}}. \tag{1.82}$$

Theorem 1.5.12 (Inversion Formula). *For an integrable characteristic function ϕ_X, the probability density function of a random variable X is given as*

$$\mathbb{P}\{X \leq x\} = \frac{1}{2\pi}\int_0^x \int_{-\infty}^{\infty} e^{-its}\phi_X(t)\,\mathrm{d}t\,\mathrm{d}s.$$

Lemma 1.5.13 *For all $t \in \mathbb{R}$ and $n \in \mathbb{N}$,*

$$\left| e^{it} - \sum_{k=0}^{n-1} \frac{(it)^k}{k!} \right| \leq \frac{|t|^n}{n!}. \tag{1.83}$$

For the next results, we need to describe the concept of convergence for the sequences of random variables.

Definition 1.5.14 *A sequence $\{X_n\}_{n\in\mathbb{N}}$ of random variables*

- *converges **in probability** to a random variable X, i.e. $X_n \xrightarrow{\mathrm{P}} X$, if*

$$\lim_{n\to\infty} \mathbb{P}[|X_n - X| > \varepsilon] = 0 \quad \text{for all } \varepsilon > 0. \tag{1.84}$$

- *converges **almost everywhere** or **almost surely** to a random variable X, i.e. $X_n \xrightarrow{\mathrm{as}} X$, if*

$$\mathbb{P}[X_n \to X] = 1. \tag{1.85}$$

- *converges **in distribution** to a random variable X, i.e. $X_n \xrightarrow{\mathrm{D}} X$, if*

$$\lim_{n\to\infty} F_{X_n}(t) = F_X(t) \tag{1.86}$$

  for all points t at which the distribution function F_X is continuous.

Remark 1.5.15 *For a sequence of random variables $\{X_n\}_{n\in\mathbb{N}}$, almost sure convergence implies convergence in probability and convergence in probability implies convergence in distribution.*

Theorem 1.5.16 (Slutsky's Theorem). *If $\{X_n\}_{n\in\mathbb{N}}$ and $\{Y_n\}_{n\in\mathbb{N}}$ are two sequences of random variables such that X_n converges in distribution to X and Y_n converges in probability to a constant C, then*

$$X_n + Y_n \xrightarrow{\mathrm{D}} X + C$$

and

$$X_n Y_n \xrightarrow{\mathrm{D}} XC,$$

provided that their sums and products are well defined.

Definition 1.5.17 *Let $\{X_1, X_2, \dots, X_N\}$ be a sample of N random variables. Then a U-statistic, stands for unbiased statistics, is defined as*

$$U_N := \frac{1}{\binom{N}{a}} \sum \dots \sum_{1\le i_1<\dots i_a\le N} h(X_{i_1}, \dots, X_{i_a}), \quad N \ge a, \tag{1.87}$$

where $h : \mathbb{R}^a \to \mathbb{R}$, $a \in \mathbb{N}$ is a measurable function which is symmetric in its arguments. The unbiasedness of U_N follows from the fact that it is the average of $\binom{N}{a}$ terms.

Remark 1.5.18 *The function h in Definition 1.5.17 is called j-degenerate, if for each $x_1, x_2, \dots, x_j$*

$$\mathbb{E}[h(x_1, x_2, \dots, x_j, X_{j+1}, \dots, X_N)] = 0, \tag{1.88}$$

where $x_1, x_2, \dots, x_j$ are arbitrary fixed vectors and the expectation is taken with respect to the random variables X_k.

Definition 1.5.19 *A U-statistics with a 1-degenerate function h is called a degenerate U-statistics.*

Theorem 1.5.20 (Strong Law of Large Numbers). *Let $X_1, X_2, \dots$ be pairwise i.i.d. random variables with $\mathbb{E}|X_i| < \infty$. Further, suppose $\mathbb{E}(X_i) = \mu$ and $S_n := X_1 + X_2 + \dots + X_n$, then $S_n/n \to \mu$ almost surely as $n \to \infty$.*

Theorem 1.5.21 (Central Limit Theorem). *Let $X_1, X_2, \dots$ be pairwise i.i.d. random variables with $\mathbb{E}|X_i^2| < \infty$ and $\mathbb{E}(X_i) = 0$. Suppose $S_n := X_1 + X_2 + \dots + X_n$, σ^2 be the variance and Z be a standard normal variable. Then $S_n/\sigma\sqrt{n}$ converges in distribution to Z.*

Chapter 2

Quadrature Points on the Ball

The theory of equidistribution is a widely discussed and numerically explored topic. The problem of distributing points on a domain has a long history. Apart from the domains like circle, sphere and cube, the distribution of points on a ball has also found many applications in various fields with a focus on the applications in geosciences and medicine. There are many configurations of points available specifically on the surface of the ball (see, for e.g. [14, 31, 57, 60]), but only a few work has been done for the whole ball (see [7, 34]). In [7], the random distribution of points is discussed by defining a reproducing kernel Hilbert space on $\mathbb{R}^{d+1}$ as the tensor product of two reproducing kernels defined on the unit sphere Ω^d and on $[0, \infty[$, respectively. This approach follows similar objectives with, however, differences in the considered problem and the methodology.
Specifically, the equidistribution problem on the ball $\mathcal{B}_R$ is to find $\omega_N = \{x_1, x_2, \ldots, x_N\}$, a set of points on $\mathcal{B}_R$, such that they are uniformly distributed in $\mathcal{B}_R$. The way how uniformity can be defined is certainly not unique. We will introduce here an approach which is suitable for the case where the orthonormal basis functions $\{G^{\mathrm{X}}_{m,n,j}\}_{m,n\in\mathbb{N}_0;\, j=1,\ldots,2n+1}$ play a role in the application. Mainly, this chapter focuses on the derivation of a quantifying criterion, based on a pseudodifferential operator, for the comparison of grids.

2.1 Pseudodifferential Operators on the Ball

In this section, we introduce the concept of pseudodifferential operators on the ball $\mathcal{B}_R$. We also construct a pseudodifferential operator for the functions on the ball $\mathcal{B}_R$ and then we study its properties.
For the construction of a pseudodifferential operator on the ball, we use two

differential operators, where one acts on the angular part and the other one acts on the radial part. For the angular part, we start as in [14], with the operator $\widetilde{\mathbb{B}}$. This operator is comprised of the Beltrami operator (1.4) and is defined as follows

$$\widetilde{\mathbb{B}} := \left((-2\Delta^*) \left(-\Delta^* + \frac{1}{4} \right)^{1/2} \right). \tag{2.1}$$

For $n \in \mathbb{N}_0$, $j = 1, 2, \ldots, 2n+1$ each spherical harmonic is an eigenfunction of the operator $\widetilde{\mathbb{B}}$ corresponding to the eigenvalues $(2n+1)n(n+1)$. Moreover, we define $\widetilde{\mathbb{B}}^\ell$, an operator with the symbol

$$\left(\widetilde{\mathbb{B}}^\ell\right)^\wedge (n) := \left(2n(n+1) \left(n + \frac{1}{2} \right) \right)^\ell, \quad \ell \in \mathbb{N},$$

for the angular part. For $p \in \mathbb{R}$ and a Sobolev space H_s on the sphere Ω (see, for e.g. [13, 24, 47]), we give the following definition.

Definition 2.1.1 *For s, $p \in \mathbb{R}$ with $s \geq 3p$, we define an operator*

$$\widetilde{\mathbb{B}}^p : H_s(\Omega) \to H_{s-3p}(\Omega)$$

by its eigenvalues

$$\left(\widetilde{\mathbb{B}}^p\right)^\wedge (n) := ((2n+1)n(n+1))^p \tag{2.2}$$

corresponding to the spherical harmonics $Y_{n,j}$.

An advantage of using this specific operator is: this operator with particular values of p gives closed representations for the angular part and is, consequently, helpful for the computational purpose.
Since $\widetilde{\mathbb{B}}^p$ is not invertible, we use a modified operator $\mathbb{B}^p$, defined by its eigenvalues

$$(\mathbb{B}^p)^\wedge (n) := \begin{cases} 1, & n = 0 \\ [(2n+1)n(n+1)]^p, & n = 1, 2, \ldots \end{cases} \tag{2.3}$$

In other words, $\mathbb{B}^p$ acts on the angular part of a function F on $\mathcal{B}_R$ in the sense that

$$\mathbb{B}^p F(r\cdot) = \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} (\mathbb{B}^p)^\wedge (n) \langle F(r\cdot), Y_{n,j} \rangle_{\mathrm{L}^2(\Omega)} Y_{n,j}$$

with respect to $\mathrm{L}^2(\Omega)$ and for (almost) every $r \in [0, R]$. Next, we proceed to the operators acting on the radial dependence. We already know from [2, 47, 50] that the operator

$$\mathbb{D}^{\mathrm{X}} := \left(-D^{\mathrm{X}} + \frac{9}{4} \right), \tag{2.4}$$

corresponding to the eigenvalues

$$\left(-D^{\mathrm{I}} + \frac{9}{4} \right)^{\wedge} (m,n) = \left(l_n + 2m + \frac{3}{2} \right)^2, \quad \mathrm{X} = \mathrm{I} \tag{2.5}$$

$$\left(-D^{\mathrm{II}} + \frac{9}{4} \right)^{\wedge} (m,n) = \left(m + \frac{3}{2} \right)^2, \quad \mathrm{X} = \mathrm{II} \tag{2.6}$$

is the differential operator of

$$P_m^{(0,l_n+\frac{1}{2})} \left(2 \left(\frac{r}{R} \right)^2 - 1 \right) \left(\frac{r}{R} \right)^{l_n}$$

for $\mathrm{X} = \mathrm{I}$ and

$$P_m^{(0,2)} \left(2\frac{r}{R} - 1 \right)$$

for $\mathrm{X} = \mathrm{II}$, respectively. This means, for $\mathrm{X} = \mathrm{I}$

$$\begin{aligned} &\left(-D^{\mathrm{I}} + \frac{9}{4} \right) P_m^{(0,l_n+\frac{1}{2})} \left(2 \left(\frac{r}{R} \right)^2 - 1 \right) \left(\frac{r}{R} \right)^{l_n} \\ &\quad = \left(l_n + 2m + \frac{3}{2} \right)^2 P_m^{(0,l_n+\frac{1}{2})} \left(2 \left(\frac{r}{R} \right)^2 - 1 \right) \left(\frac{r}{R} \right)^{l_n}, \end{aligned}$$

where $\left(-D^{\mathrm{I}} + \frac{9}{4}\right)^{\wedge}(m,n) = \left(l_n + 2m + \frac{3}{2}\right)^2 \neq 0$ for all $m, n \in \mathbb{N}_0$. In addition, using induction, we get

$$\left(\left(-D^{\mathrm{I}} + \frac{9}{4} \right)^{\ell} \right)^{\wedge} (m,n) = \left(l_n + 2m + \frac{3}{2} \right)^{2\ell}, \quad \ell \in \mathbb{N}.$$

Likewise, for $\mathrm{X} = \mathrm{II}$, we have

$$\left(\left(-D^{\mathrm{II}} + \frac{9}{4} \right)^{\ell} \right)^{\wedge} (m,n) = \left(m + \frac{3}{2} \right)^{2\ell}, \quad \ell \in \mathbb{N}.$$

This allows us to state the following definition for the operator functioning on the radial part.

Definition 2.1.2 *For any $q \in \mathbb{R}$, we define an operator $\left(\mathbb{D}^{\mathrm{X}}\right)^q := \left(-D^{\mathrm{X}} + \frac{9}{4}\right)^q$ by its eigenvalues*

$$\left(\left(-D^{\mathrm{I}} + \frac{9}{4}\right)^q\right)^\wedge (m,n) = \left(l_n + 2m + \frac{3}{2}\right)^{2q}, \quad \mathrm{X} = \mathrm{I} \tag{2.7}$$

and

$$\left(\left(-D^{\mathrm{II}} + \frac{9}{4}\right)^q\right)^\wedge (m) = \left(m + \frac{3}{2}\right)^{2q}, \quad \mathrm{X} = \mathrm{II}. \tag{2.8}$$

It is easy to see that the composition of the operators $\mathbb{B}^p$ and $\left(\mathbb{D}^{\mathrm{X}}\right)^q$ for $\mathrm{X} = \mathrm{I}$ and $\mathrm{X} = \mathrm{II}$, respectively, is again an invertible differential operator, and the following result holds true.

Theorem 2.1.3 *The operators defined by $\mathbb{A}_{\mathrm{X}}^{p,q} := \mathbb{B}^p \circ \left(\mathbb{D}^{\mathrm{X}}\right)^q$ are invertible differential operators with eigenvalues*

$$(\mathbb{A}_{\mathrm{I}}^{p,q})^\wedge(m,n) = \begin{cases} \left(l_0 + 2m + \frac{3}{2}\right)^{2q}, & n = 0,\ m \in \mathbb{N}_0 \\ \left(l_n + 2m + \frac{3}{2}\right)^{2q} [(2n+1)n(n+1)]^p, & n \in \mathbb{N},\ m \in \mathbb{N}_0 \end{cases} \tag{2.9}$$

corresponding to the orthonormal system

$$G_{m,n,j}^{\mathrm{I}}(x) = \sqrt{\frac{4m + 2l_n + 3}{R^3}} P_m^{(0, l_n + \frac{1}{2})}\left(2\frac{|x|^2}{R^2} - 1\right) \left(\frac{|x|}{R}\right)^{l_n} Y_{n,j}\left(\frac{x}{|x|}\right),$$

$x \in \mathcal{B}_R \setminus \{0\}$, $m, n \in \mathbb{N}_0$; $j = 1, 2, ..., 2n+1$, and

$$(\mathbb{A}_{\mathrm{II}}^{p,q})^\wedge(m,n) = \begin{cases} \left(m + \frac{3}{2}\right)^{2q}, & n = 0,\ m \in \mathbb{N}_0 \\ \left(m + \frac{3}{2}\right)^{2q} [(2n+1)n(n+1)]^p, & n \in \mathbb{N},\ m \in \mathbb{N}_0 \end{cases} \tag{2.10}$$

corresponding to the orthonormal system

$$G_{m,n,j}^{\mathrm{II}}(x) = \sqrt{\frac{2m+3}{R^3}} P_m^{(0,2)}\left(2\frac{|x|}{R} - 1\right) Y_{n,j}\left(\frac{x}{|x|}\right),$$

$x \in \mathcal{B}_R \setminus \{0\}$, $m, n \in \mathbb{N}_0$; $j = 1, 2, ..., 2n+1$, where $\mathbb{B}^p$ is defined by (2.3) and $\left(\mathbb{D}^{\mathrm{X}}\right)^q$ is defined by (2.7) and (2.8) for $\mathrm{X} = \mathrm{I}$ and $\mathrm{X} = \mathrm{II}$, respectively.

Proof: By the definition of the operators $\mathbb{A}_{\mathrm{X}}^{p,q}$, we have

$$\begin{aligned} (\mathbb{A}_{\mathrm{X}}^{p,q})^\wedge (m,n) &= \left(\mathbb{B}^p \circ \left(\mathbb{D}^{\mathrm{X}}\right)^q\right)^\wedge (m,n) \\ &= (\mathbb{B}^p)^\wedge (n) \left(\left(\mathbb{D}^{\mathrm{X}}\right)^q\right)^\wedge (m,n). \end{aligned}$$

Now, the result is an immediate consequence of Definition 2.1.2 and Equation (2.3). ■

Based on the sequences (2.9) and (2.10), we now define particular Sobolev spaces.

Definition 2.1.4 *For $s,t \in \mathbb{R}_0^+$, consider the sequences defined in (2.9) and (2.10) for $p = s$ and $q = t/2$, then we define a Sobolev space depending on them as*

$$\mathcal{H}_{s,t}^{\mathrm{X}}(\mathcal{B}_R) := \mathcal{H}\left(\left\{\left(\mathbb{A}_{\mathrm{X}}^{s,\frac{t}{2}}\right)^{\wedge}(m,n)\right\}, \mathrm{X}, \mathcal{B}_R\right). \tag{2.11}$$

Proposition 2.1.5 *For all $s_1, s_2, t_1, t_2 \in \mathbb{R}_0^+$ with $s_1 \geq s_2$ and $t_1 \geq t_2$, we have*

$$\mathcal{H}_{s_1,t_1}^{\mathrm{X}}(\mathcal{B}_R) \subset \mathcal{H}_{s_2,t_2}^{\mathrm{X}}(\mathcal{B}_R).$$

The above sequences are X-summable if they satisfy (1.63) and (1.64) for types I and II, respectively, i.e.

$$\sum_{m,n=0}^{\infty} \left(\left(\mathbb{A}_{\mathrm{I}}^{s,\frac{t}{2}}\right)^{\wedge}(m,n)\right)^{-2} (2n+1)(4m+2l_n+3)\frac{(l_n+m+\frac{1}{2})^{2m}}{(m!\,)^2} < +\infty,$$

and

$$\sum_{m,n=0}^{\infty} \left(\left(\mathbb{A}_{\mathrm{II}}^{s,\frac{t}{2}}\right)^{\wedge}(m,n)\right)^{-2} (2n+1)(2m+3)^5 < +\infty.$$

Hence, due to the Sobolev lemma (see Lemma 1.4.7), every function $F \in \mathcal{H}_{s,t}^{\mathrm{X}}(\mathcal{B}_R)$, for a summable sequence, has a uniformly convergent Fourier series on $\mathcal{B}_R$ and is continuous on $\mathcal{B}_R\backslash\{0\}$. With the use of Remark 1.4.8, F is also continuous on $\mathcal{B}_R$ for type I with $l_n = n$. Since $\mathcal{H}_{s,t}^{\mathrm{X}}(\mathcal{B}_R)$ is a reproducing kernel Hilbert space (see Chapter 1), we denote the corresponding reproducing kernel here by $K_{\mathcal{H}_{s,t}^{\mathrm{X}}}$.

Theorem 2.1.6 *The sequence $\{(\mathbb{A}_{\mathrm{II}}^{s,\frac{t}{2}})^{\wedge}(m,n)\}_{m,n\in\mathbb{N}_0}$ defined in* (2.10) *is a* II*-summable sequence for $s > \frac{1}{3}$ and $t > 3$.*

Proof: Because of its decoupling (of radial and angular parts) property, it is easy to see that the sequence (2.10) is of the order of $\mathcal{O}(n^{3s}m^t)$ and is, therefore, II-summable for $s > \frac{1}{3}$ and $t > 3$. ■

This structure of Sobolev spaces helps us to introduce a general notation for the pseudodifferential operators on $\mathcal{B}_R$ in analogy to the spherical concept in [24].

Definition 2.1.7 *For $s,t \in \mathbb{R}_0^+$ with $s \geq \frac{p}{3}$ and $t \geq q$, the operator*

$$\mathcal{A} : \mathcal{H}_{s,t}^{\mathrm{X}}(\mathcal{B}_R) \to \mathcal{H}_{s-\frac{p}{3},t-q}^{\mathrm{X}}(\mathcal{B}_R)$$

defined as

$$\mathcal{A}F = \sum_{m,n=0}^{\infty}\sum_{j=1}^{2n+1} A_{m,n} \left\langle F, G_{m,n,j}^{\mathrm{X}}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} G_{m,n,j}^{\mathrm{X}}$$

is called a pseudodifferential operator of type I *with respect to the orthonormal system of type* I*, if, for all* $m, n \in \mathbb{N}_0$*, the corresponding eigenvalues* $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ *satisfy*

$$c_1(n+c_2)^p(l_n+2m+c_3)^q \leq |A_{m,n}| \leq c_4(n+c_5)^p(l_n+2m+c_6)^q, \qquad (2.12)$$

where the Fourier coefficients $\left\langle F, G^{\mathrm{X}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)}$ *vanish for all* $l_n < 0$ *(see Definition 1.4.5). Also,* $\mathcal{A}$ *is named as a pseudodifferential operator of type* II*, if, for all* $m, n \in \mathbb{N}_0$*,* $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ *satisfy*

$$c_1(n+c_2)^p(m+c_3)^q \leq |A_{m,n}| \leq c_4(n+c_5)^p(m+c_6)^q, \qquad (2.13)$$

where $c_i > 0$ *are fixed and* $p, q \in \mathbb{R}^+_0$ *are respectively called the angular and radial orders of the operator.*

We will now derive the properties of the pseudodifferential operators.

Lemma 2.1.8 *Let* P *and* Q *be polynomials of degree* d_1 *and* d_2*, respectively, with* d_1 *and* $d_2 \in \mathbb{N}$*. Further, let* $P(n) > 0$ *and* $Q(n) > 0$ *for all* $n \in I = [c, +\infty[$ *with fixed* $c \in \mathbb{R}$*. Then the following holds true: For a sequence* $\{P(n)^i\}_{n\in I}$ *with an arbitrary but fixed* $i \in \mathbb{R}^+$*, there exists a constant* b_i*, which depends on* i*, such that*

$$P(n)^i \leq b_i\, Q(n)^{i\frac{d_1}{d_2}}$$

for all $n \in I$*.*

Proof: Let $a_n := \frac{P(n)^{d_2}}{Q(n)^{d_1}}$ for all $n \in I$ and let γ and $\tilde{\gamma}$ be the leading coefficients of P and Q, respectively, that is

$$P(x) = \gamma\, x^{d_1} + \mathcal{O}(x^{d_1-1}), \quad Q(x) = \tilde{\gamma}\, x^{d_2} + \mathcal{O}(x^{d_2-1}), \quad \text{as } x \to \infty.$$

The conditions on P and Q imply that $\gamma, \tilde{\gamma} \in \mathbb{R}^+$. Furthermore,

$$\lim_{n\to\infty} a_n = \frac{\gamma^{d_2}}{\tilde{\gamma}^{d_1}} > 0.$$

Thus, there exists $n_0 \in I$ such that, for all $n \geq n_0$, $a_n \leq 2\frac{\gamma^{d_2}}{\tilde{\gamma}^{d_1}}$. Now let $b := \max\left\{\max_{n\in[c,n_0]} a_n, 2\frac{\gamma^{d_2}}{\tilde{\gamma}^{d_1}}\right\}$. Then, we have

$$a_n \leq b$$

and, consequently,

$$P(n)^i \leq b^{\frac{i}{d_2}}\, Q(n)^{i\frac{d_1}{d_2}} \tag{2.14}$$

for all $n \in I$. With $b_i := b^{\frac{i}{d_2}}$, we have the desired result. ■

In order to see that $\mathcal{A}F$, indeed, maps into the Sobolev space $\mathcal{H}^{\mathrm{I}}_{s-\frac{p}{3},t-q}(\mathcal{B}_R)$, we consider

$$\begin{aligned}\|\mathcal{A}F\|^2_{\mathcal{H}^{\mathrm{I}}_{s-\frac{p}{3},t-q}(\mathcal{B}_R)} &= \sum_{m,n=0}^{\infty}\sum_{j=1}^{2n+1}\left[\left(\mathbb{A}_{\mathrm{I}}^{s-\frac{p}{3},\frac{t-q}{2}}\right)^{\wedge}(m,n)\left\langle \mathcal{A}F, G^{\mathrm{I}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)}\right]^2\\ &= \sum_{m,n=0}^{\infty}\sum_{j=1}^{2n+1}\left[\left(\mathbb{A}_{\mathrm{I}}^{s-\frac{p}{3},\frac{t-q}{2}}\right)^{\wedge}(m,n)A_{m,n}\left\langle F, G^{\mathrm{I}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)}\right]^2.\end{aligned}$$

We use (2.9) and (2.12) in the above equation and arrive at

$$\begin{aligned}&\|\mathcal{A}F\|^2_{\mathcal{H}^{\mathrm{I}}_{s-\frac{p}{3},t-q}(\mathcal{B}_R)}\\ &= \sum_{m=0}^{\infty}\left[\left(\mathbb{A}_{\mathrm{I}}^{s-\frac{p}{3},\frac{t-q}{2}}\right)^{\wedge}(m,0)A_{m,0}\left\langle F, G^{\mathrm{I}}_{m,0,1}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)}\right]^2\\ &\quad+\sum_{m=0}^{\infty}\sum_{n=1}^{\infty}\sum_{j=1}^{2n+1}\left[\left(\mathbb{A}_{\mathrm{I}}^{s-\frac{p}{3},\frac{t-q}{2}}\right)^{\wedge}(m,n)A_{m,n}\left\langle F, G^{\mathrm{I}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)}\right]^2\\ &\leq \sum_{m=0}^{\infty}\left[\left(l_0+2m+\frac{3}{2}\right)^{t-q}c_4\,c_5^p\,(l_0+2m+c_6)^q\left\langle F, G^{\mathrm{I}}_{m,0,1}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)}\right]^2\\ &\quad+\sum_{m=0}^{\infty}\sum_{n=1}^{\infty}\sum_{j=1}^{2n+1}\left[\left(l_n+2m+\frac{3}{2}\right)^{t-q}[(2n+1)n(n+1)]^{s-\frac{p}{3}}\right.\\ &\qquad\left.\times c_4(n+c_5)^p(l_n+2m+c_6)^q\left\langle F, G^{\mathrm{I}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)}\right]^2.\end{aligned}$$

It should be noted here that for the case $l_n < 0$, the Fourier coefficients $\left\langle F, G^{\mathrm{I}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)}$ vanish for all corresponding (m,n,j) (see Definition 1.4.5). Now, using Lemma 2.1.8, we can find constants a and b depending on q and p, such that

$$(n+c_5)^p \leq a\,((2n+1)n(n+1))^{\frac{p}{3}}$$

and

$$(l_n+2m+c_6)^q \leq b\left(l_n+2m+\frac{3}{2}\right)^q$$

for all $m, n \geq 0$. Note that the second inequality is obtained, if $k := l_n + 2m$ is used as an index of the sequence. So, there exist positive constants C^* and C^{**} such that

$$\begin{aligned} \|\mathcal{A}F\|^2_{\mathcal{H}^{\mathrm{I}}_{s-\frac{p}{3},t-q}(\mathcal{B}_R)} &\leq C^* \sum_{m=0}^{\infty} \left[\left(l_0 + 2m + \frac{3}{2} \right)^t \left\langle F, G^{\mathrm{I}}_{m,0,1} \right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} \right]^2 \\ &\quad + C^{**} \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \Bigg[\left(l_n + 2m + \frac{3}{2} \right)^t ((2n+1)n(n+1))^s \\ &\qquad \times \left\langle F, G^{\mathrm{I}}_{m,n,j} \right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} \Bigg]^2 \\ &\leq C \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} \left[\left(\mathbb{A}_{\mathrm{I}}^{s,\frac{t}{2}} \right)^{\wedge} (m,n) \left\langle F, G^{\mathrm{I}}_{m,n,j} \right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} \right]^2 \\ &< +\infty, \end{aligned}$$

where $C = \max(C^*, C^{**})$. Similarly, we have

$$\|\mathcal{A}F\|^2_{\mathcal{H}^{\mathrm{II}}_{s-\frac{p}{3},t-q}(\mathcal{B}_R)} < +\infty.$$

This proves the following result.

Theorem 2.1.9 *The operator $\mathcal{A}$ defined in Definition 2.1.7, indeed, has the property that*

$$\mathcal{A}\left(\mathcal{H}^{\mathrm{X}}_{s,t}(\mathcal{B}_R)\right) \subset \mathcal{H}^{\mathrm{X}}_{s-\frac{p}{3},t-q}(\mathcal{B}_R).$$

In particular, we also get a result for the domain and the order of the operators in Theorem 2.1.3.

Theorem 2.1.10 *For $s, t, p, q \in \mathbb{R}^+_0$ with $s \geq p$ and $t \geq 2q$, the operator*

$$\mathbb{A}^{p,q}_{\mathrm{X}} : \mathcal{H}^{\mathrm{X}}_{s,t}(\mathcal{B}_R) \to \mathcal{H}^{\mathrm{X}}_{s-p,t-2q}(\mathcal{B}_R)$$

defined in Theorem 2.1.3 is a pseudodifferential operator with the angular order $3p$ and radial order $2q$. Moreover, the operator is isometric, that is

$$\|\mathbb{A}^{p,q}_{\mathrm{X}}(F)\|_{\mathcal{H}^{\mathrm{X}}_{s-p,t-2q}(\mathcal{B}_R)} = \|F\|_{\mathcal{H}^{\mathrm{X}}_{s,t}(\mathcal{B}_R)}, \quad F \in \mathcal{H}^{\mathrm{X}}_{s,t}(\mathcal{B}_R).$$

In particular, for the case $s = p$ and $t = 2q$

$$\left\|\mathbb{A}^{s,\frac{t}{2}}_{\mathrm{X}}(F)\right\|_{\mathrm{L}^2(\mathcal{B}_R)} = \|F\|_{\mathcal{H}^{\mathrm{X}}_{s,t}(\mathcal{B}_R)}, \quad F \in \mathcal{H}^{\mathrm{X}}_{s,t}(\mathcal{B}_R).$$

Proof: The statement of $\mathbb{A}_{\mathrm{X}}^{p,q}$ being a pseudodifferential operator with given radial and angular orders is guaranteed by Lemma 2.1.8. Further, in order to prove the isometry of the operator, we consider the norm of $F \in \mathcal{H}_{s,t}^{\mathrm{X}}(\mathcal{B}_R)$ for $s \geq p$, $t \geq 2q$ and get

$$
\begin{aligned}
&\|\mathbb{A}_{\mathrm{X}}^{p,q}(F)\|^2_{\mathcal{H}^{\mathrm{X}}_{s-p,t-2q}(\mathcal{B}_R)} \\
&\quad = \sum_{m,n=0}^{\infty} \sum_{j=1}^{2n+1} \left[\left(\mathbb{A}_{\mathrm{X}}^{s-p,\frac{t}{2}-q} \right)^{\wedge} (m,n) \left\langle \mathbb{A}_{\mathrm{X}}^{p,q}(F), G^{\mathrm{X}}_{m,n,j} \right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} \right]^2 \\
&\quad = \sum_{m,n=0}^{\infty} \sum_{j=1}^{2n+1} \left[\left(\mathbb{A}_{\mathrm{X}}^{s-p,\frac{t}{2}-q} \right)^{\wedge} (m,n) \left(\mathbb{A}_{\mathrm{X}}^{p,q}\right)^{\wedge} (m,n) \left\langle F, G^{\mathrm{X}}_{m,n,j} \right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} \right]^2 \\
&\quad = \sum_{m,n=0}^{\infty} \sum_{j=1}^{2n+1} \left[\left(\mathbb{A}_{\mathrm{X}}^{s,\frac{t}{2}} \right)^{\wedge} (m,n) \left\langle F, G^{\mathrm{X}}_{m,n,j} \right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} \right]^2 \\
&\quad = \|F\|^2_{\mathcal{H}^{\mathrm{X}}_{s,t}(\mathcal{B}_R)} .
\end{aligned}
$$

This completes the proof. ■

2.2 Generalized Discrepancy

Principally, a quadrature formula depends on two quantities that are: the weights and the grid points. First, we consider a quadrature formula with fixed equal weights and search for a set $\omega_N = \{x_1, x_2, \ldots, x_N\} \subset \mathcal{B}_R$, such that

$$
\int_{\mathcal{B}_R} F(x)\,\mathrm{d}x \approx \frac{4\pi R^3}{3N} \sum_{k=1}^{N} F(x_k) \tag{2.15}
$$

for any function $F \in \mathcal{H}(\mathcal{B}_R)$. We now derive an estimate for the quadrature error.

Theorem 2.2.1 *For any function $F \in \mathcal{H}(\{B_{m,n}\}, \mathrm{X}, \mathcal{B}_R)$, we have*

$$
\begin{aligned}
&\left| \frac{3}{4\pi R^3} \int_{\mathcal{B}_R} F(x)\,\mathrm{d}x - \frac{1}{N} \sum_{k=1}^{N} F(x_k) \right| \\
&\quad \leq \|\mathcal{A}F\|_{\mathrm{L}^2(\mathcal{B}_R)} \frac{1}{N} \left[\sum_{\substack{(m,n)\neq(0,0) \\ A_{m,n}\neq 0}} \sum_{j=1}^{2n+1} \sum_{i=1}^{N} \sum_{k=1}^{N} \frac{G^{\mathrm{X}}_{m,n,j}(x_i) G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}} \right]^{\frac{1}{2}} ,
\end{aligned} \tag{2.16}
$$

where the Sobolev space $\mathcal{H}(\{B_{m,n}\}, \mathrm{X}, \mathcal{B}_R)$ *depends on a summable sequence* $\{B_{m,n}\}_{m,n\in\mathbb{N}_0}$ *and* $\mathcal{A} : \mathcal{H}(\{B_{m,n}\}, \mathrm{X}, \mathcal{B}_R) \to \mathrm{L}^2(\mathcal{B}_R)$ *is an operator with summable eigenvalues* $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ *such that* $A_{m,n} = 0$ *if and only if* $B_{m,n} = 0$ *and* $A_{0,0} \neq 0$.

Proof: Let us consider $F \in \mathcal{H}(\{B_{m,n}\}, \mathrm{X}, \mathcal{B}_R)$, then we can write

$$\begin{aligned} F(y) &= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\sum_{j=1}^{2n+1} \left\langle F, G^{\mathrm{X}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} G^{\mathrm{X}}_{m,n,j}(y) \\ &= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\sum_{j=1}^{2n+1} \int_{\mathcal{B}_R} F(x) G^{\mathrm{X}}_{m,n,j}(x)\,\mathrm{d}x\, G^{\mathrm{X}}_{m,n,j}(y) \end{aligned}$$

for all $y \in \mathcal{B}_R$, since for a summable sequence this expansion is uniformly convergent (see Lemma 1.4.7). Separating the term for $(m,n) = (0,0)$, we get

$$F(y) = \frac{3}{4\pi R^3}\int_{\mathcal{B}_R} F(x)\,\mathrm{d}x + \sum_{(m,n)\neq(0,0)}\sum_{j=1}^{2n+1}\int_{\mathcal{B}_R} F(x) G^{\mathrm{X}}_{m,n,j}(x)\,\mathrm{d}x\, G^{\mathrm{X}}_{m,n,j}(y).$$

For any operator $\mathcal{A}$ with eigenvalues $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$, the equation above becomes

$$F(y) = \frac{3}{4\pi R^3}\int_{\mathcal{B}_R} F(x)\,\mathrm{d}x + \sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}}\sum_{j=1}^{2n+1}\int_{\mathcal{B}_R} \frac{\mathcal{A}F(x) G^{\mathrm{X}}_{m,n,j}(x)}{A_{m,n}}\,\mathrm{d}x\, G^{\mathrm{X}}_{m,n,j}(y).$$

Next, putting $y = x_k$ and taking a sum over all indices $k \in \{1, 2, \ldots, N\}$, we obtain

$$\begin{aligned} &\frac{1}{N}\sum_{k=1}^{N} F(x_k) \\ &= \frac{3}{4\pi R^3}\int_{\mathcal{B}_R} F(x)\,\mathrm{d}x + \sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}}\sum_{j=1}^{2n+1}\int_{\mathcal{B}_R} \frac{\mathcal{A}F(x) G^{\mathrm{X}}_{m,n,j}(x)}{A_{m,n}}\,\mathrm{d}x\, \frac{1}{N}\sum_{k=1}^{N} G^{\mathrm{X}}_{m,n,j}(x_k). \end{aligned}$$

Now the error estimate is calculated as:

$$\begin{aligned} &\left| \frac{3}{4\pi R^3}\int_{\mathcal{B}_R} F(x)\,\mathrm{d}x - \frac{1}{N}\sum_{k=1}^{N} F(x_k)\right| \\ &= \left| \sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}}\sum_{j=1}^{2n+1}\int_{\mathcal{B}_R} \frac{\mathcal{A}F(x) G^{\mathrm{X}}_{m,n,j}(x)}{A_{m,n}}\,\mathrm{d}x\, \frac{1}{N}\sum_{k=1}^{N} G^{\mathrm{X}}_{m,n,j}(x_k)\right|. \end{aligned}$$

Considering the uniform convergence of the series, we can interchange the integral and summation and get

$$\left| \frac{3}{4\pi R^3} \int_{\mathcal{B}_R} F(x)\,\mathrm{d}x - \frac{1}{N} \sum_{k=1}^{N} F(x_k) \right|$$
$$= \left| \frac{1}{N} \int_{\mathcal{B}_R} \mathcal{A}F(x) \sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}} \sum_{j=1}^{2n+1} \frac{G^{\mathrm{X}}_{m,n,j}(x)}{A_{m,n}} \sum_{k=1}^{N} G^{\mathrm{X}}_{m,n,j}(x_k)\,\mathrm{d}x \right|.$$

Furthermore, using the Cauchy-Schwarz inequality (1.17), we obtain

$$\left| \frac{3}{4\pi R^3} \int_{\mathcal{B}_R} F(x)\,\mathrm{d}x - \frac{1}{N} \sum_{k=1}^{N} F(x_k) \right|$$
$$\leq \frac{1}{N} \left(\int_{\mathcal{B}_R} (\mathcal{A}F(x))^2\,\mathrm{d}x \right)^{\frac{1}{2}} \left(\int_{\mathcal{B}_R} \left(\sum_{\substack{(m,n)\\ \neq(0,0)}} \sum_{\substack{j=1\\ A_{m,n}\neq 0}}^{2n+1} \sum_{k=1}^{N} \frac{G^{\mathrm{X}}_{m,n,j}(x) G^{\mathrm{X}}_{m,n,j}(x_k)}{A_{m,n}} \right)^2 \mathrm{d}x \right)^{\frac{1}{2}}.$$

We know that, from Sobolev lemma 1.4.7, the second term in the above inequality, i.e. $K_{\mathcal{H}}(\cdot, x_k) \in \mathrm{C}(\mathcal{B}_R)$ and, consequently, is in $\mathrm{L}^2(\mathcal{B}_R)$. This yields

$$\left| \frac{3}{4\pi R^3} \int_{\mathcal{B}_R} F(x)\,\mathrm{d}x - \frac{1}{N} \sum_{k=1}^{N} F(x_k) \right|$$
$$= \frac{1}{N} \|\mathcal{A}F\|_{\mathrm{L}^2(\mathcal{B}_R)} \left(\sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}} \sum_{j=1}^{2n+1} \left(\sum_{k=1}^{N} \frac{G^{\mathrm{X}}_{m,n,j}(x_k)}{A_{m,n}} \right)^2 \right)^{\frac{1}{2}}$$
$$= \frac{1}{N} \|\mathcal{A}F\|_{\mathrm{L}^2(\mathcal{B}_R)} \left(\sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}} \sum_{j=1}^{2n+1} \sum_{i=1}^{N} \sum_{k=1}^{N} \frac{G^{\mathrm{X}}_{m,n,j}(x_i) G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}} \right)^{\frac{1}{2}},$$

which is the required quadrature error estimate. ■

This error estimate allows us to describe the generalized discrepancy for the ball.

Definition 2.2.2 *The generalized discrepancy $D(\omega_N, \mathcal{A})$ for the ball depending on the operator $\mathcal{A}$ with the symbol $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ and a point grid $\omega_N = \{x_1, x_2, \ldots, x_N\}$ is defined as*

$$D(\omega_N, \mathcal{A}) := \frac{1}{N}\left(\sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}} \sum_{j=1}^{2n+1}\sum_{i=1}^{N}\sum_{k=1}^{N} \frac{G^{\mathrm{X}}_{m,n,j}(x_i)G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}}\right)^{\frac{1}{2}}. \tag{2.17}$$

The generalized discrepancy acts as a uniformity measure for the points distributed on the ball. The lower the discrepancy is, the more the points are equidistributed.

Definition 2.2.3 *If the generalized discrepancy converges to zero for large N, i.e. $\lim_{N\to\infty} D(\omega_N, \mathcal{A}) = 0$ for a sequence of point sets $\{\omega_N\}_{N\in\mathbb{N}}$, then $\{\omega_N\}_{N\in\mathbb{N}}$ is named as $\mathcal{A}$-equidistributed in the Sobolev space $\mathcal{H}(\mathcal{B}_R)$.*

2.3 Weighted Grid Point Approximation

Unlike the concept given in the previous section, the weighted grid point approximation estimates the integral of the functions on the given domain using nonuniform weights. In this section, we analyse the integral of the functions on the ball using variable weights instead of the constant ones. We can reframe the problem in the following way: taking a set of points ω_N on the ball $\mathcal{B}_R$, we need to search for the weights α_k such that

$$\int_{\mathcal{B}_R} F(x)\,\mathrm{d}x \approx \frac{4\pi R^3}{3}\sum_{k=1}^{N}\alpha_k F(x_k),$$

for any function $F \in \mathcal{H}(\mathcal{B}_R)$. For any operator $\mathcal{A}$ on $\mathcal{H}(\mathcal{B}_R)$ with summable eigenvalues $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$, we can conclude the following:

Theorem 2.3.1 *Let $\omega_N = \{x_1, x_2, \ldots, x_N\}$ be a fixed point set on $\mathcal{B}_R$ and $\{\alpha_1, \alpha_2, \ldots, \alpha_N\}$ be weights such that*

$$\sum_{k=1}^{N}\alpha_k = 1.$$

Then for any function $F \in \mathcal{H}(\{B_{m,n}\}, \mathrm{X}, \mathcal{B}_R)$*, we have*

$$\left| \frac{3}{4\pi R^3} \int_{\mathcal{B}_R} F(x)\,\mathrm{d}x - \sum_{k=1}^{N} \alpha_k F(x_k) \right|$$
$$\leq \|\mathcal{A}F\|_{\mathrm{L}^2(\mathcal{B}_R)} \left[\sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}} \sum_{j=1}^{2n+1} \sum_{i=1}^{N} \sum_{k=1}^{N} \frac{\alpha_i \alpha_k G^{\mathrm{X}}_{m,n,j}(x_i) G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}} \right]^{\frac{1}{2}}, \tag{2.18}$$

where the Sobolev space $\mathcal{H}(\{B_{m,n}\}, \mathrm{X}, \mathcal{B}_R)$ *depends on a summable sequence* $\{B_{m,n}\}_{m,n\in\mathbb{N}_0}$ *and* $\mathcal{A} : \mathcal{H}(\{B_{m,n}\}, \mathrm{X}, \mathcal{B}_R) \to \mathrm{L}^2(\mathcal{B}_R)$ *is an operator with summable eigenvalues* $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ *such that* $A_{m,n} = 0$ *if and only if* $B_{m,n} = 0$ *and* $A_{0,0} \neq 0$.

Proof: The result can be proved using the same procedure as in Theorem 2.2.1. ■

Based on this result, we now define the weighted discrepancy.

Definition 2.3.2 *The weighted discrepancy* $D_{\mathrm{w}}(\omega_N, \mathcal{A})$ *depending on the operator* $\mathcal{A}$ *with the symbol* $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ *and* N *weights* $\alpha_1, \alpha_2, \ldots, \alpha_N$ *satisfying*

$$\sum_{k=1}^{N} \alpha_k = 1 \tag{2.19}$$

is defined as

$$D_{\mathrm{w}}(\omega_N, \mathcal{A}) := \left[\sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}} \sum_{j=1}^{2n+1} \sum_{i=1}^{N} \sum_{k=1}^{N} \frac{\alpha_i \alpha_k G^{\mathrm{X}}_{m,n,j}(x_i) G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}} \right]^{\frac{1}{2}}. \tag{2.20}$$

Now we have to find the weights in order to have a minimum discrepancy for a specific set of points on the ball. This gives rise to an optimization problem in which the function to be minimized is $D_{\mathrm{w}}(\omega_N, \mathcal{A})$. The problem is stated as: we minimize the term

$$Q_{\mathcal{A}}(\alpha_1, \alpha_2, \ldots, \alpha_N) = \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_i \alpha_k h(\mathcal{A}; x_i, x_k),$$

where

$$h(\mathcal{A}; x_i, x_k) = \sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}} \sum_{j=1}^{2n+1} \frac{G^{\mathrm{X}}_{m,n,j}(x_i) G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}}$$

subject to the constraints

$$\sum_{k=1}^{N} \alpha_k = 1.$$

To minimize our objective function $Q_{\mathcal{A}}$ subject to the given constraints, we use the Lagrange method of multipliers with Lagrange multiplier λ. The Lagrange function in this case is given as

$$L(\alpha_1, \alpha_2, \ldots, \alpha_N, \lambda) = Q_{\mathcal{A}}(\alpha_1, \alpha_2, \ldots, \alpha_N) - \lambda \left(\sum_{k=1}^{N} \alpha_k - 1 \right). \tag{2.21}$$

Next, taking the partial derivatives of (2.21) with respect to the variables α_t, $t = 1, 2, \ldots, N$ and the new variable λ, we get the following system of equations to be solved:

$$\begin{aligned} h(\mathcal{A}; x_1, x_1)\alpha_1 + h(\mathcal{A}; x_2, x_1)\alpha_2 + \ \ldots\ + h(\mathcal{A}; x_N, x_1)\alpha_N - \frac{\lambda}{2} &= 0 \\ h(\mathcal{A}; x_1, x_2)\alpha_1 + h(\mathcal{A}; x_2, x_2)\alpha_2 + \ \ldots\ + h(\mathcal{A}; x_N, x_2)\alpha_N - \frac{\lambda}{2} &= 0 \\ &\vdots \\ h(\mathcal{A}; x_1, x_N)\alpha_1 + h(\mathcal{A}; x_2, x_N)\alpha_2 + \ \ldots\ + h(\mathcal{A}; x_N, x_N)\alpha_N - \frac{\lambda}{2} &= 0 \\ \alpha_1 + \alpha_2 + \ \ldots\ + \alpha_N - 1 &= 0. \end{aligned} \tag{2.22}$$

Now multiplying the first N equations by α_t for $t = 1, 2, \ldots, N$ and taking sum over indices t, we have

$$\sum_{t=1}^{N} \sum_{i=1}^{N} h(\mathcal{A}; x_i, x_t)\alpha_i\alpha_t - \frac{\lambda}{2} \underbrace{\sum_{t=1}^{N} \alpha_t}_{=1} = 0.$$

Consequently, we get

$$\sum_{t=1}^{N} \sum_{i=1}^{N} h(\mathcal{A}; x_i, x_t)\alpha_i\alpha_t = \frac{\lambda}{2}. \tag{2.23}$$

This leads us to the following result.

Theorem 2.3.3 *If λ is the Lagrange multiplier and $D_{\mathrm{w}}(\omega_N, \mathcal{A})$ is the weighted discrepancy with optimum weights α_k satisfying* (2.19)*, then we have*

$$D_{\mathrm{w}}(\omega_N, \mathcal{A}) = \left(\frac{\lambda}{2} \right)^{\frac{1}{2}}. \tag{2.24}$$

2.4 Operators and Eigenvalues

The choice of the sequence $\{B_{m,n}\}_{m,n\in\mathbb{N}_0}$ and the operator $\mathcal{A}$ with its eigenvalues $A_{m,n}$ satisfying the conditions of Theorem 2.2.1, in the generalized discrepancy (2.17) and the weighted discrepancy (2.20) is not restricted. Here, we work with the Sobolev spaces $\mathcal{H}^{\mathrm{X}}_{s,t}(\mathcal{B}_R)$ (see Definition 2.1.4) and further experiment with different sequences $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ in order to get a convenient representation of the discrepancy formula. With the use of the orthonormal system of type I given by (1.50) for $R = 1$ and the addition theorem for spherical harmonics 1.3.11, (2.20) yields

$$D_{\mathrm{w}}(\omega_N, \mathcal{A}) = \left[\sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}} \sum_{i=1}^{N}\sum_{k=1}^{N} \frac{\alpha_i\alpha_k}{4\pi} \frac{(2n+1)(4m+2l_n+3)}{A^2_{m,n}} \left(|x_i||x_k|\right)^{l_n} \times P_m^{(0,l_n+\frac{1}{2})}(2|x_i|^2-1) P_m^{(0,l_n+\frac{1}{2})}(2|x_k|^2-1) P_n\left(\xi_i\cdot\xi_k\right)\right]^{\frac{1}{2}}, \quad (2.25)$$

where $\xi_i := \frac{x_i}{|x_i|}$. Similarly, for the orthonormal system of type II (1.51) with $R = 1$, we have

$$D_{\mathrm{w}}(\omega_N, \mathcal{A}) = \left[\sum_{\substack{(m,n)\neq(0,0)\\ A_{m,n}\neq 0}} \sum_{i=1}^{N}\sum_{k=1}^{N} \frac{\alpha_i\alpha_k}{4\pi} \frac{(2n+1)(2m+3)}{A^2_{m,n}} P_m^{(0,2)}(2|x_i|-1) \times P_m^{(0,2)}(2|x_k|-1) P_n\left(\xi_i\cdot\xi_k\right)\right]^{\frac{1}{2}}. \quad (2.26)$$

Note that for $\alpha_i = \alpha_k = \frac{1}{N}$, $D_{\mathrm{w}}(\omega_N, \mathcal{A}) = D(\omega_N, \mathcal{A})$. In the following, we discuss some examples of the sequences $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ together with the representations of the discrepancy formula in these particular cases. The most convenient choice for eigenvalues is, of course, the sequences (2.9) and (2.10) which we have also chosen for the Sobolev spaces $\mathcal{H}^{\mathrm{X}}_{s,t}(\mathcal{B}_R)$. Note that the summability condition for sequences (see Definition 1.4.6) is only sufficient and there are more cases where the Sobolev lemma 1.4.7 holds. In what follows, we consider the cases with suitable values of p and q.

- $\mathcal{A} := \mathbb{A}^{p,q}_{\mathrm{I}}$ and $A_{m,n} := \left(\mathbb{A}^{p,q}_{\mathrm{I}}\right)^{\wedge}(m,n)$

For the sequence (2.9) with sufficiently large p and q, (2.25) becomes

$$D_{\mathrm{w}}\left(\omega_N, \mathbb{A}_{\mathrm{I}}^{p,q}\right) = \left[\sum_{m=1}^{\infty}\sum_{i,k=1}^{N} \frac{\alpha_i\alpha_k}{2\pi} \frac{2m+l_0+\frac{3}{2}}{(2m+l_0+\frac{3}{2})^{4q}} \right.$$
$$\times P_m^{(0,l_0+\frac{1}{2})}(2|x_i|^2-1) P_m^{(0,l_0+\frac{1}{2})}(2|x_k|^2-1) \left(|x_i||x_k|\right)^{l_0} P_0\left(\xi_i\cdot\xi_k\right)$$
$$+ \sum_{m=0}^{\infty}\sum_{n=1}^{\infty}\sum_{i,k=1}^{N} \frac{\alpha_i\alpha_k}{2\pi} \frac{(2n+1)(2m+l_n+\frac{3}{2})}{(2m+l_n+\frac{3}{2})^{4q}[(2n+1)n(n+1)]^{2p}}$$
$$\left.\times P_m^{(0,l_n+\frac{1}{2})}(2|x_i|^2-1) P_m^{(0,l_n+\frac{1}{2})}(2|x_k|^2-1) \left(|x_i||x_k|\right)^{l_n} P_n\left(\xi_i\cdot\xi_k\right)\right]^{\frac{1}{2}}.$$

Writing it down in a compact form, we arrive at

$$D_{\mathrm{w}}\left(\omega_N, \mathbb{A}_{\mathrm{I}}^{p,q}\right) = \left[\sum_{m=1}^{\infty}\sum_{i,k=1}^{N} \frac{\alpha_i\alpha_k}{2\pi} \frac{1}{\left(\mathbb{A}_{\mathrm{I}}^{2p,2q-\frac{1}{2}}\right)^{\wedge}(m,0)} P_m^{(0,l_0+\frac{1}{2})}(2|x_i|^2-1) \right.$$
$$\times P_m^{(0,l_0+\frac{1}{2})}(2|x_k|^2-1) \left(|x_i||x_k|\right)^{l_0} P_0\left(\xi_i\cdot\xi_k\right)$$
$$+ \sum_{m=0}^{\infty}\sum_{n=1}^{\infty}\sum_{i,k=1}^{N} \frac{\alpha_i\alpha_k}{2\pi} \frac{2n+1}{\left(\mathbb{A}_{\mathrm{I}}^{2p,2q-\frac{1}{2}}\right)^{\wedge}(m,n)} P_m^{(0,l_n+\frac{1}{2})}(2|x_i|^2-1)$$
$$\left.\times P_m^{(0,l_n+\frac{1}{2})}(2|x_k|^2-1) \left(|x_i||x_k|\right)^{l_n} P_n\left(\xi_i\cdot\xi_k\right)\right]^{\frac{1}{2}}.$$

This leads us to the following equation:

$$D_{\mathrm{w}}\left(\omega_N, \mathbb{A}_{\mathrm{I}}^{p,q}\right) = \left[\sum_{\substack{m=0 \\ (m,n)\neq(0,0)}}^{\infty}\sum_{n=0}^{\infty}\sum_{i,k=1}^{N} \frac{\alpha_i\alpha_k}{2\pi} \frac{2n+1}{\left(\mathbb{A}_{\mathrm{I}}^{2p,2q-\frac{1}{2}}\right)^{\wedge}(m,n)} \right.$$
$$\left.\times P_m^{(0,l_n+\frac{1}{2})}(2|x_i|^2-1) P_m^{(0,l_n+\frac{1}{2})}(2|x_k|^2-1) \left(|x_i||x_k|\right)^{l_n} P_n\left(\xi_i\cdot\xi_k\right)\right]^{\frac{1}{2}}.$$

Furthermore, subtracting the term with indices $(m,n) = (0,0)$, we obtain

$$D_{\mathrm{w}}\left(\omega_N, \mathbb{A}_{\mathrm{I}}^{p,q}\right) = \left[\sum_{m,n=0}^{\infty}\sum_{i,k=1}^{N} \frac{\alpha_i\alpha_k}{2\pi} \frac{2n+1}{\left(\mathbb{A}_{\mathrm{I}}^{2p,2q-\frac{1}{2}}\right)^{\wedge}(m,n)} P_m^{(0,l_n+\frac{1}{2})}(2|x_i|^2-1)\right.$$
$$\left. \times P_m^{(0,l_n+\frac{1}{2})}(2|x_k|^2-1)\left(|x_i||x_k|\right)^{l_n} P_n\left(\xi_i\cdot\xi_k\right) - \frac{\alpha_i\alpha_k}{2\pi}\frac{\left(|x_i||x_k|\right)^{l_0}}{\left(\mathbb{A}_{\mathrm{I}}^{2p,2q-\frac{1}{2}}\right)^{\wedge}(0,0)}\right]^{\frac{1}{2}}. \tag{2.27}$$

- $\mathcal{A} := \mathbb{A}_{\mathrm{II}}^{p,q}$ and $A_{m,n} := \left(\mathbb{A}_{\mathrm{II}}^{p,q}\right)^{\wedge}(m,n)$
  Like before, for the sequence (2.10) with sufficiently large p and q, equation (2.26) becomes

$$D_{\mathrm{w}}\left(\omega_N, \mathbb{A}_{\mathrm{II}}^{p,q}\right) = \left[\sum_{m,n=0}^{\infty}\sum_{i,k=1}^{N} \frac{\alpha_i\alpha_k}{2\pi} \frac{2n+1}{\left(\mathbb{A}_{\mathrm{II}}^{2p,2q-\frac{1}{2}}\right)^{\wedge}(m,n)}\right.$$
$$\left. \times P_m^{(0,2)}(2|x_i|-1)P_m^{(0,2)}(2|x_k|-1)P_n\left(\xi_i\cdot\xi_k\right) - \frac{\alpha_i\alpha_k}{2\pi}\frac{1}{\left(\mathbb{A}_{\mathrm{II}}^{2p,2q-\frac{1}{2}}\right)^{\wedge}(0,0)}\right]^{\frac{1}{2}}. \tag{2.28}$$

In particular, for $p = \frac{1}{2}$ and $q = \frac{3}{4}$, the above equation takes the form

$$D_{\mathrm{w}}\left(\omega_N, \mathbb{A}_{\mathrm{II}}^{\frac{1}{2},\frac{3}{4}}\right) = \frac{1}{\sqrt{\pi}}\left[\sum_{i=1}^{N}\sum_{k=1}^{N}\sum_{m=0}^{\infty}\frac{2\alpha_i\alpha_k}{(2m+3)^2}P_m^{(0,2)}(2|x_i|-1)\right.$$
$$\left. \times\ P_m^{(0,2)}(2|x_k|-1)\left(1+\sum_{n=1}^{\infty}\frac{1}{n(n+1)}P_n\left(\xi_i\cdot\xi_k\right)\right) - \frac{2}{9}\alpha_i\alpha_k\right]^{\frac{1}{2}}. \tag{2.29}$$

For this sequence, we get a closed representation for the angular part as (see [44])

$$\sum_{n=1}^{\infty}\frac{1}{n(n+1)}P_n\left(\xi_i\cdot\xi_k\right) = 1 - 2\ln\left(1+\sqrt{\frac{1-\xi_i\cdot\xi_k}{2}}\right),$$

which is actually the reason behind choosing these particular values of

p and q. Hence, the discrepancy in this case takes the form

$$D_{\mathrm{w}}\left(\omega_N, \mathbb{A}_{\mathrm{II}}^{\frac{1}{2},\frac{3}{4}}\right) = \sqrt{\frac{2}{\pi}}\left[\sum_{i=1}^{N}\sum_{k=1}^{N}\sum_{m=0}^{\infty}\frac{2\alpha_i\alpha_k}{(2m+3)^2}P_m^{(0,2)}(2|x_i|-1)\right.$$
$$\left.\times\ P_m^{(0,2)}(2|x_k|-1)\left(1-\ln\left(1+\sqrt{\frac{1-\xi_i\cdot\xi_k}{2}}\right)\right)-\frac{1}{9}\alpha_i\alpha_k\right]^{\frac{1}{2}}. \quad (2.30)$$

Note that the sequence (2.10) with $p = \frac{1}{2}$ and $q = \frac{3}{4}$ is not summable, however, the summability is a sufficient and not necessary condition for our considerations. The conditions in Theorem 2.2.1 allow us to choose this particular operator, where we can take a truncation of series over m for the numerical relevance.

Apart from selecting these specific differential operators together with their eigenvalues, we can also choose other (summable) sequences. Specifically, we can find different representations for the discrepancy D_{w} in (2.26) corresponding to a specific sequence, as it completely decouples the m and n parts which are related to the angular and radial parts of the orthonormal basis system of type II. Obviously, this cannot be done for the discrepancy D_{w} in (2.25) which depends on the orthonormal system of type I. Fortunately, we have some closed representations for the angular part which helps us in the numerical calculations. The following sequences can be chosen according to some representations for the angular part.

- $A_{m,n} := \sqrt{\left(\frac{2m+3}{2t^m}\frac{2n+1}{2t^n}\right)}$, $0 < t < 1$
  For the above sequence, (2.26) takes the form

$$D_{\mathrm{w}}(\omega_N, \mathcal{A}) = \left[\sum_{i,k=1}^{N}\frac{\alpha_i\alpha_k}{\pi}\left(\sum_{m=0}^{\infty}t^m P_m^{(0,2)}(2|x_i|-1)P_m^{(0,2)}(2|x_k|-1)\right)\right.$$
$$\left.\times\left(\sum_{n=0}^{\infty}t^n P_n(\xi_i\cdot\xi_k)\right)-\frac{\alpha_i\alpha_k}{\pi}\right]^{\frac{1}{2}}.$$

With

$$\sum_{n=0}^{\infty}t^n P_n(\xi_i\cdot\xi_k) = \frac{1}{\sqrt{1+t^2-2t\xi_i\cdot\xi_k}}$$

(see [53]), the above equation yields

$$D_{\mathrm{w}}\left(\omega_N,\mathcal{A}\right)=\left[\sum_{i,k=1}^{N}\frac{\alpha_i\alpha_k}{\pi}\left(\sum_{m=0}^{\infty}t^m P_m^{(0,2)}(2|x_i|-1)P_m^{(0,2)}(2|x_k|-1)\right)\right.$$
$$\left.\times\frac{1}{\sqrt{1+t^2-2t\xi_i\cdot\xi_k}}-\frac{\alpha_i\alpha_k}{\pi}\right]^{\frac{1}{2}}. \quad (2.31)$$

- $A_{m,n}:=\sqrt{\frac{2m+3}{4t^m t^n}}$, $0<t<1$
  For the above sequence, (2.26) takes the form

$$D_{\mathrm{w}}\left(\omega_N,\mathcal{A}\right)=\left[\sum_{i,k=1}^{N}\frac{\alpha_i\alpha_k}{\pi}\left(\sum_{m=0}^{\infty}t^m P_m^{(0,2)}(2|x_i|-1)P_m^{(0,2)}(2|x_k|-1)\right)\right.$$
$$\left.\times\left(\sum_{n=0}^{\infty}(2n+1)t^n P_n\left(\xi_i\cdot\xi_k\right)\right)-\frac{\alpha_i\alpha_k}{\pi}\right]^{\frac{1}{2}}.$$

With the representation

$$\sum_{n=0}^{\infty}(2n+1)t^n P_n(\xi_i\cdot\xi_k)=\frac{1-t^2}{(1+t^2-2t\xi_i\cdot\xi_k)^{\frac{3}{2}}}$$

for the n part (see [53]), the discrepancy is given as

$$D_{\mathrm{w}}\left(\omega_N,\mathcal{A}\right)=\left[\sum_{i,k=1}^{N}\frac{\alpha_i\alpha_k}{\pi}\left(\sum_{m=0}^{\infty}t^m P_m^{(0,2)}(2|x_i|-1)P_m^{(0,2)}(2|x_k|-1)\right)\right.$$
$$\left.\times\frac{1-t^2}{(1+t^2-2t\xi_i\cdot\xi_k)^{\frac{3}{2}}}-\frac{\alpha_i\alpha_k}{\pi}\right]^{\frac{1}{2}}. \quad (2.32)$$

- $A_{m,n}:=\sqrt{\frac{2m+3}{2t^m}\frac{(2n+1)(n+1)}{2t^n}}$, $0<t<1$
  In analogy to above, using the representation

$$\sum_{n=0}^{\infty}\frac{t^n}{n+1}P_n(\xi_i\cdot\xi_k)=\frac{1}{t}\ln\left[\frac{t-\xi_i\cdot\xi_k+\sqrt{1-2t\xi_i\cdot\xi_k+t^2}}{1-\xi_i\cdot\xi_k}\right]$$

for the n part (see [44]) and the given sequence $A_{m,n}$, we have

$$D_{\mathrm{w}}\left(\omega_N, \mathcal{A}\right) = \left[\sum_{i,k=1}^{N} \frac{\alpha_i\alpha_k}{\pi} \left(\sum_{m=0}^{\infty} t^m P_m^{(0,2)}(2|x_i|-1) P_m^{(0,2)}(2|x_k|-1)\right)\right.$$
$$\left. \times \frac{1}{t} \ln\left(\frac{t - \xi_i \cdot \xi_k + \sqrt{1 - 2t\xi \cdot \xi_k + t^2}}{1 - \xi_i \cdot \xi_k}\right) - \frac{\alpha_i\alpha_k}{\pi}\right]^{\frac{1}{2}}. \quad (2.33)$$

Note that the operators $\mathcal{A}$ corresponding to all sequences $A_{m,n}$ are pseudodifferential operators and are defined as

$$\mathcal{A}F = A_{m,n}F \quad \text{for all } F \in \mathcal{H}_{s,t}^{\mathrm{X}}(\mathcal{B}_R).$$

It is easy to see that the last three sequences are II-summable for all $t \in]0,1[$.

Chapter 3

Construction of Point Grids and Discrepancy Estimates

This chapter deals with the construction of the grids on a 3-dimensional ball and the computation of their discrepancies. We acquire grids on the ball with the help of known configurations on the surface of the ball. For this, we use the simple approach of plotting equidistributed spherical grids for different but equidistant radii r. Therefore, we get distribution of points not only on the surface but also inside the ball. We test four different spherical grids, that are: the simple lattice, the improved lattice, the Freeden grid and the Reuter grid. Each point grid is generated by a division of latitude and longitude. A grid on the ball is generated by using a spherical grid of different radii r. In our examples, the radius r varies from 0 to 1 with a distance of 0.1 between each spherical grid. Figures 3.1 to 3.3 show plots of the resulting grids

1. Simple Lattice [14]: This is t most famous as well as simp point grid known on the sphe which gives an equal division longitude ϕ and latitude θ. It c pends on two parameters P and where P, $Q \in \mathbb{N}$, and

$$\theta_i = \frac{i\pi}{P}, \quad 1 \leq i \leq P-1,$$
$$\phi_j = \frac{2j\pi}{Q}, \quad 1 \leq j \leq Q-1. \tag{3.1}$$

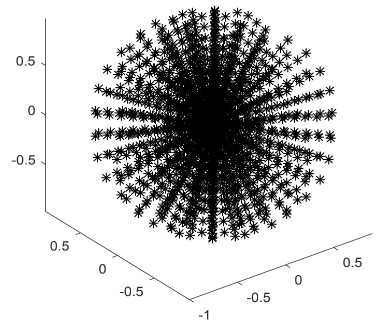


Figure 3.1: simple lattice of 1690 points on a 3D-ball.

When we plot this grid on the ball for parameters $P = Q$ using the criterion stated above, we get (.

2. Improved Lattice [14]: The i proved lattice is actually an i proved version of the simple l tice. Here, the value of the lon tude ϕ is dependent on θ due which the points do not show concentration near the poles.

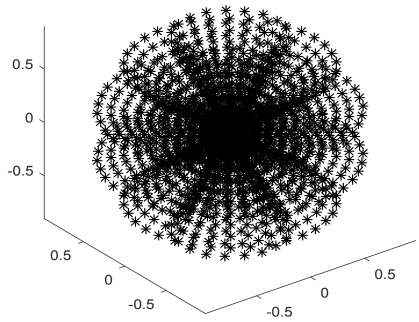


Figure 3.2: Improved lattice with 1900 points on the 3D-ball.

$$\theta_i = \frac{i\pi}{P}, \quad 1 \leq i \leq P-1,$$
$$j(i) = \lfloor 2\pi P \sin(\theta_i) \rfloor,$$
$$\phi_j = \frac{2j\pi}{j(i)}, \quad 1 \leq j \leq j(i),$$

where $\lfloor . \rfloor$ represents the Gaussian bracket. For a given parameter P, the total number of distinct points we get in this case is $\left(\sum_{i=1}^{P-1} j(i)\right)$.

3. Reuter Grid [58]: For $P \in \mathbb{N}$, we have

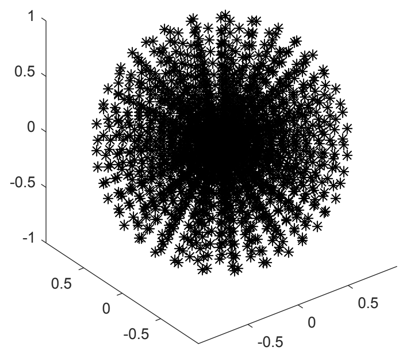


Figure 3.3: Reuter grid with 2080 points on the 3D-ball.

$$\theta_i = \frac{i\pi}{P}, \quad 0 \leq i \leq P,$$
$$\gamma_0 = 1,\ \gamma_P = 1,$$
$$\gamma_i = \left\lfloor \frac{2\pi}{\arccos\left(\frac{\cos\left(\frac{\pi}{P}\right) - \cos^2(\theta_i)}{\sin^2(\theta_i)}\right)} \right\rfloor,$$
$$1 \leq i \leq P-1,$$
$$\phi_{01} = 0,\ \phi_{P1} = 0,$$
$$\phi_{ij} = \left(j - \frac{1}{2}\right)\left(\frac{2\pi}{\gamma_i}\right), \quad 1 \leq j \leq \gamma_i,$$
$$1 \leq i \leq P-1.$$

The grid is named after the author of PhD thesis [58]. This spherical grid, when plotted on the unit ball, gives a nice distribution of points in comparison to other examples. For $P \in \mathbb{N}$, the number of points N on the surface of the ball in this case can be estimated by

$$N \leq 2 + \frac{4}{\pi} P^2.$$

4. Freeden Grid [47]: For $P \in \mathbb{N}$, we have

$$\theta_0 = 0,\ \phi_{01} = 0,$$
$$\theta_i = \frac{i\pi}{P}, \quad 1 \le i \le P-1,$$
$$i \le P/2 : \gamma_i = 4i,$$
$$i > P/2 : \gamma_i = 4(P-i),$$
$$\phi_{ij} = \left(j - \frac{1}{2}\right)\left(\frac{2\pi}{\gamma_i}\right), \quad 1 \le j \le$$
$$1 \le i \le P-1,$$
$$\theta_P = \pi,\ \phi_{P1} = 0.$$

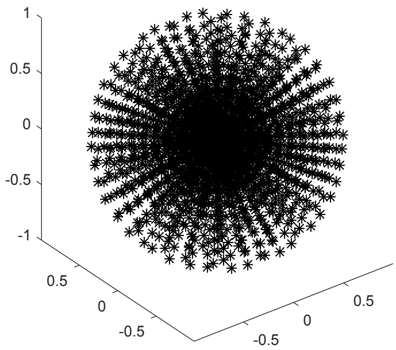


Figure 3.4: Freeden grid with 1980 points on the 3D-ball.

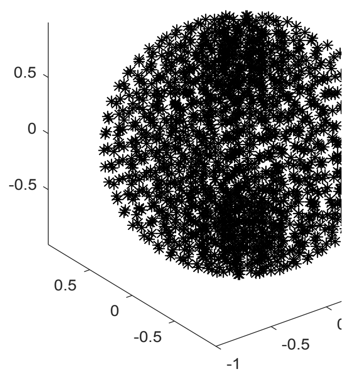
The number of points N on the surface of the ball in this case is determined by

$$N = 2 + 4\left\lfloor \frac{P+1}{2} \right\rfloor \left\lfloor \frac{P}{2} \right\rfloor.$$

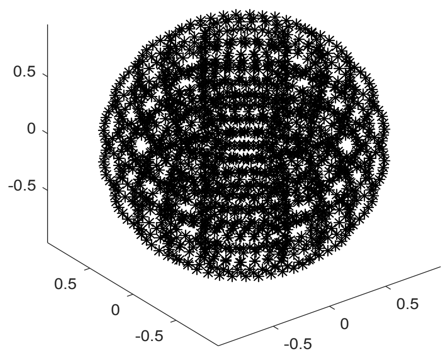
One major drawback of this construction, as it can be seen in all the examples above, is the aggregation of points at the centre of the ball. The reason is that, while plotting the grids, the same number of points is used on the spheres of different radii. As a consequence, we do not get a nice distribution of points on the ball. In the next section, we discuss a way to improve these grids in order to get comparatively finer distributions.

3.1 Modified Point Grids

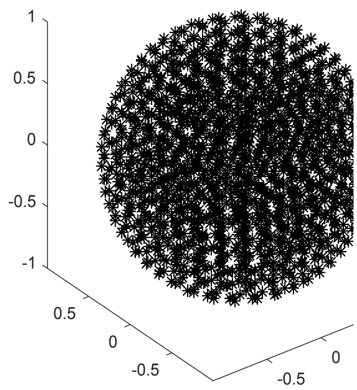
In this section, we modify the originally constructed grids in order to solve the problem of accumulation of points near the origin. We know from the previous section that every spherical grid depends on a paramter P, which gives the division of points. We replace this parameter P in the original grids by the term $\lfloor rP \rfloor$, $\lfloor . \rfloor$ representing the Gaussian bracket. This term depends on the radius r of the sphere so that with the increasing radii of the spheres, the number of points on each sphere also increases. Figures 3.5a to 3.5d show the behaviour of the point grids after the modification. A comparison to the plots obtained from the first attempt of constructing point grids on the ball shows that the modified point grids lead to better results. We can see that the points are now no more accumulated at the centre of the ball. They are also visually more equidistributed.



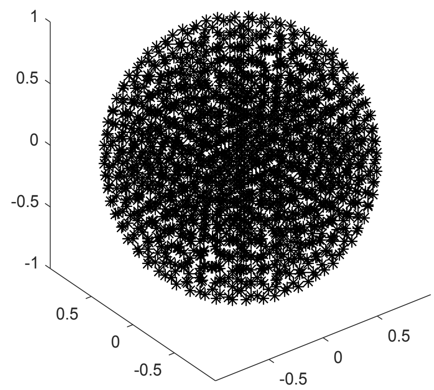
(a) A plot of the modified simple



(b) A plot of the modified improved



(c) A plot of the modified Reuter grid with 1638 grid points and a discrepancy value of 0.0604.



(d) A plot of the modified Freeden grid with 1600 grid points and a discrepancy value of 0.0590.

Figure 3.5: Plots of modified point grids on the 3D-ball.

Furthermore, one can calculate the discrepancies of these constructed grids using any of the discrepancy formulae derived in Chapter 2. In order to be brief, we use only equation (2.27) for type I and equation (2.30) for type II to compute the discrepancies with weights $\alpha_i = \frac{1}{N}$. Since the parameters m and n in (2.27) and the parameter m in (2.30) sum up to infinite values, we truncate them to degrees $\mathcal{M}$ and $\mathcal{N}$ of Jacobi and Legendre polynomials, respectively. In the following computations, we take $\mathcal{M} = 50$ and $\mathcal{N} = 50$

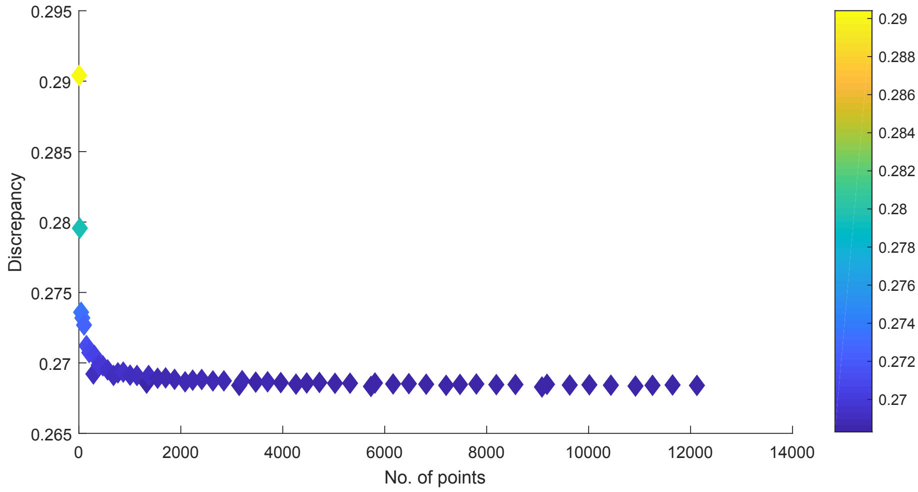
for the case of type I and for type II, we choose $\mathcal{M} = 100$.
Similar to the case of type II, we take the operator with values $p = \frac{1}{2}$ and $q = \frac{3}{4}$ for the type I also. With these particular values of p, q and $l_n = n$, (2.27) yields

$$D_{\mathrm{w}}\left(\omega_N, \mathbb{A}_{\mathrm{I}}^{\frac{1}{2},\frac{3}{4}}\right) = \left[\sum_{m=0}^{\mathcal{M}}\sum_{n=0}^{\mathcal{N}}\sum_{i,k=1}^{N} \frac{\alpha_i\alpha_k}{2\pi} \frac{2n+1}{\left(\mathbb{A}_{\mathrm{I}}^{1,1}\right)^{\wedge}(m,n)} P_m^{(0,n+\frac{1}{2})}(2|x_i|^2-1) \right.$$
$$\left. \times\, P_m^{(0,n+\frac{1}{2})}(2|x_k|^2-1)\left(|x_i||x_k|\right)^n P_n\left(\xi_i\cdot\xi_k\right) - \frac{\alpha_i\alpha_k}{2\pi}\frac{1}{\left(\mathbb{A}_{\mathrm{I}}^{1,1}\right)^{\wedge}(0,0)}\right]^{\frac{1}{2}}, \quad (3.2)$$

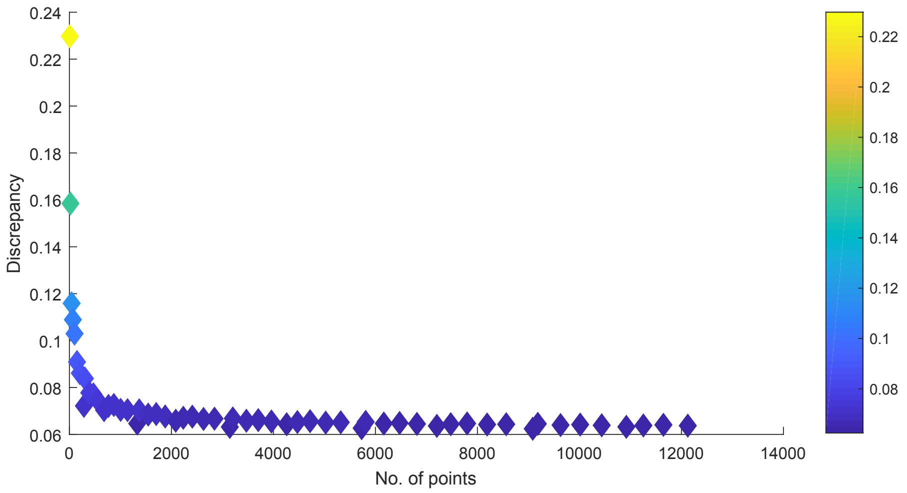
and for $\alpha_i = \frac{1}{N}$, we obtain

$$D\left(\omega_N, \mathbb{A}_{\mathrm{I}}^{\frac{1}{2},\frac{3}{4}}\right) = \left[\sum_{m=0}^{\mathcal{M}}\sum_{n=0}^{\mathcal{N}}\sum_{i,k=1}^{N} \frac{1}{2\pi N^2} \frac{2n+1}{\left(\mathbb{A}_{\mathrm{I}}^{1,1}\right)^{\wedge}(m,n)} P_m^{(0,n+\frac{1}{2})}(2|x_i|^2-1) \right.$$
$$\left. \times\, P_m^{(0,n+\frac{1}{2})}(2|x_k|^2-1)\left(|x_i||x_k|\right)^n P_n\left(\xi_i\cdot\xi_k\right) - \frac{1}{2\pi N^2}\frac{1}{\left(\mathbb{A}_{\mathrm{I}}^{1,1}\right)^{\wedge}(0,0)}\right]^{\frac{1}{2}}. \quad (3.3)$$

It is easy to see that for these values of p and q with $l_n = n$, the series in (3.3) is convergent.
From this point onwards, all the computations are done with $l_n = n$ for the case of type I. We again mention here that the value $l_n = n$ plays a particular role. For this specific value, the basis system I forms an algebraic polynomial. Moreover, it is relevant for the singular value decomposition of the inverse gravimetric problem (see, for e.g. [4, 49]).
The plots in figures 3.6 to 3.9 show the dependence of the discrepancy estimates computed for the basis systems of types I and II with respect to the number of points.

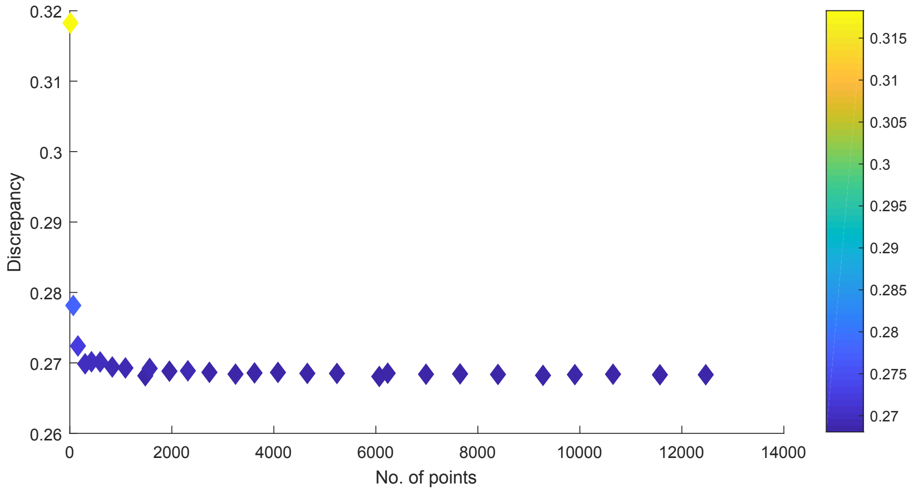


(a)

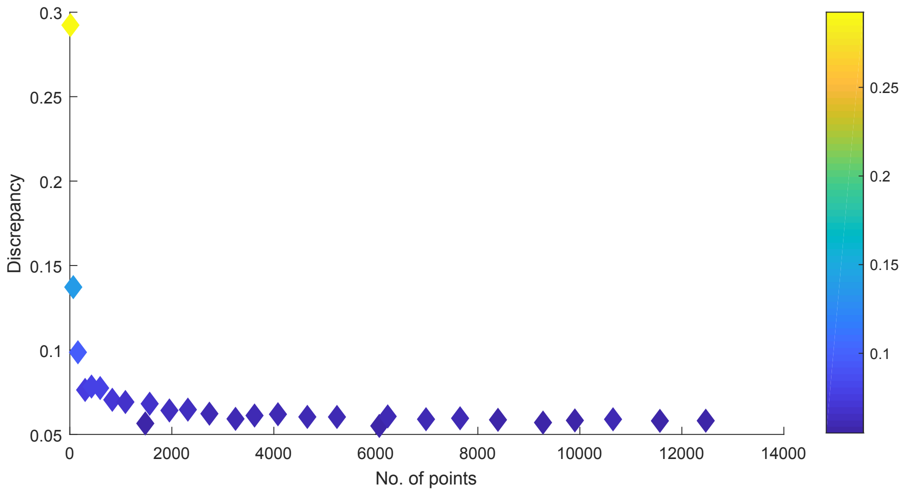


(b)

Figure 3.6: The behaviour of the generalized discrepancies with increasing number of points for the modified simple lattice corresponding to the orthonormal basis system of type I is presented in (a) and for the orthonormal basis system of type II in (b). The colourbar represents the values of the discrepancies.

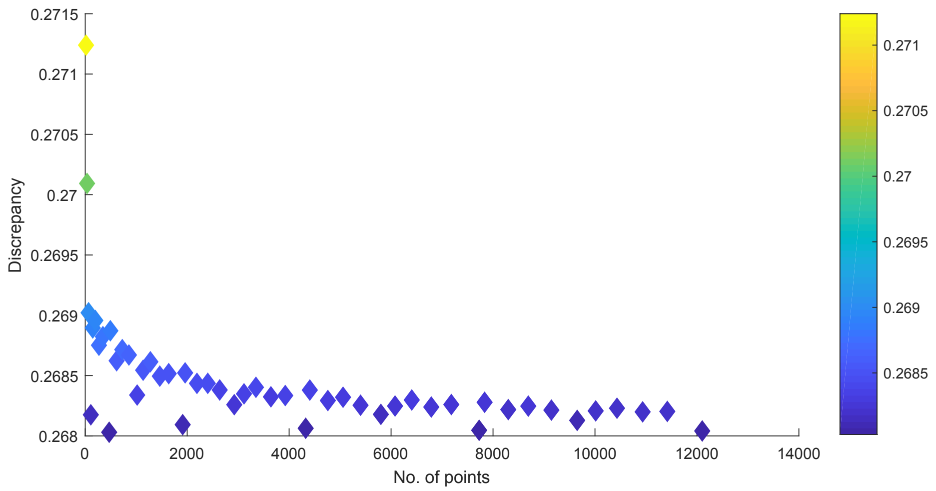


(a)

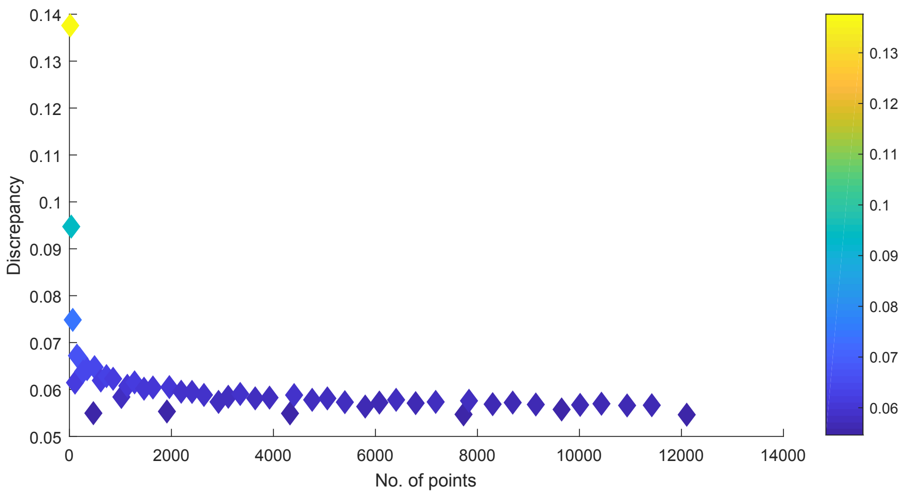


(b)

Figure 3.7: The behaviour of the generalized discrepancies with increasing number of points for the modified improved lattice corresponding to the orthonormal basis system of type I is presented in (a) and for the orthonormal basis system of type II in (b). The colourbar represents the values of the discrepancies.

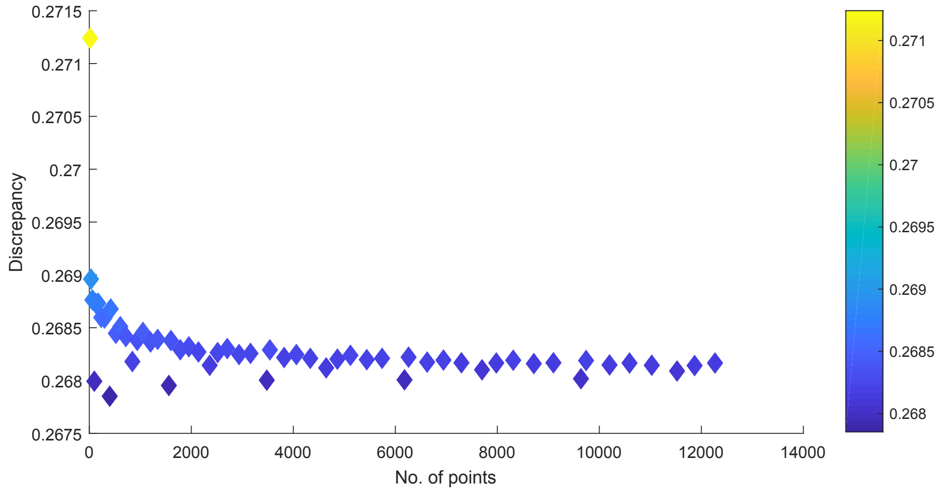


(a)

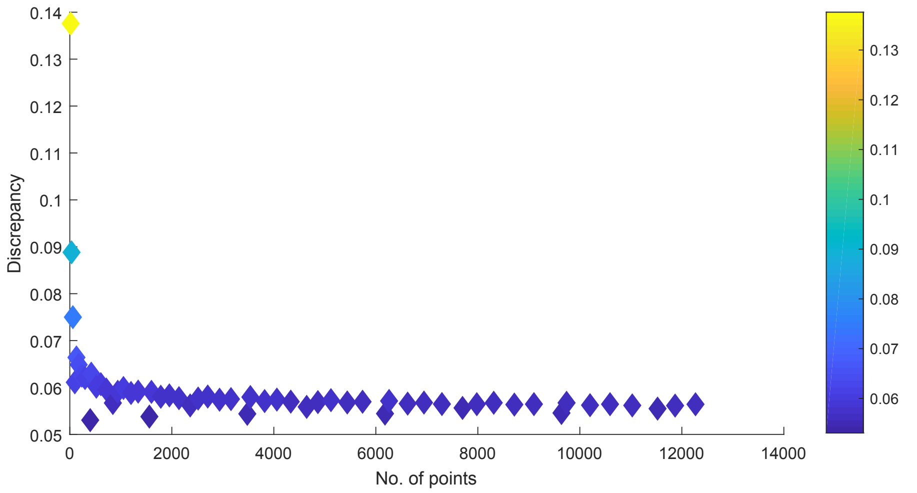


(b)

Figure 3.8: The behaviour of the generalized discrepancies with increasing number of points for the modified Reuter grid corresponding to the orthonormal basis system of type I is presented in (a) and for the orthonormal basis system of type II in (b). The colourbar represents the values of the discrepancies.



(a)



(b)

Figure 3.9: The behaviour of the generalized discrepancies with increasing number of points for the modified Freeden grid corresponding to the orthonormal basis system of type I is presented in (a) and for type II in (b). The colourbar represents the values of the discrepancies.

Note that the discrepancy in all the above examples appears to stagnate for large numbers of grids and the rate of convergence is not very good but it is noticeable that the general trend of discrepancy estimates with respect to the number of points is decreasing. It can also be seen that the rate of convergence for type II is faster in comparison to type I. As mentioned above, it is also evident from the plots that Reuter grid has better outcomes among other grids for both the cases of type I and II.

3.2 Weighted Discrepancy Estimates

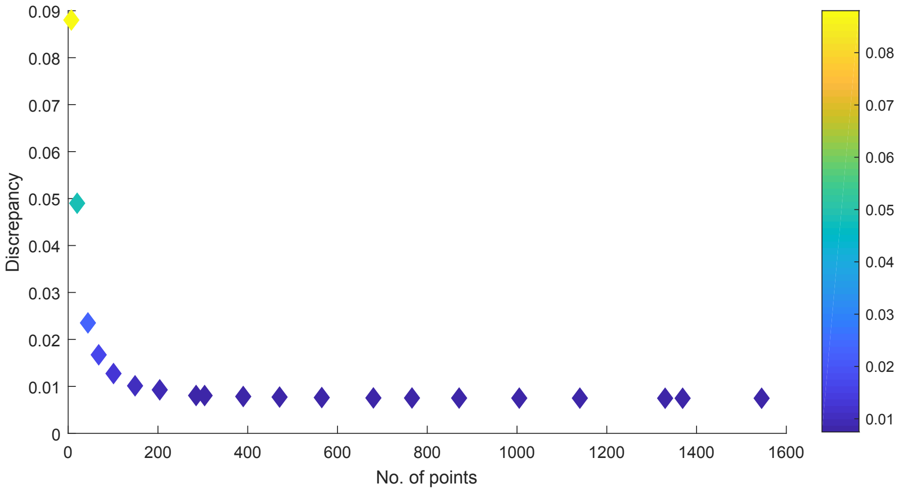
In what follows, we present the results for the weighted discrepancies in Figures 3.10 to 3.13. These discrepancies are calculated for the modified point grids from the previous section. As mentioned in Section 2.3, we choose a particular grid on the ball and search for the weights that minimize the discrepancy of that grid. In order to solve this optimization problem, we use the Lagrange method of multipliers with Lagrange multiplier λ. We solve the linear system of equations (2.22) for the variables α_k and the Lagrange multiplier λ. Firstly, for a chosen point grid $\{x_1, x_2, \ldots, x_N\}$, we calculate the value of the kernel

$$h(\mathcal{A}; x_i, x_k) = \sum_{\substack{m=0 \\ (m,n)\neq(0,0)}}^{\mathcal{M}} \sum_{n=0}^{\mathcal{N}} \sum_{j=1}^{2n+1} \frac{G^{\mathrm{X}}_{m,n,j}(x_i) G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}} \tag{3.4}$$

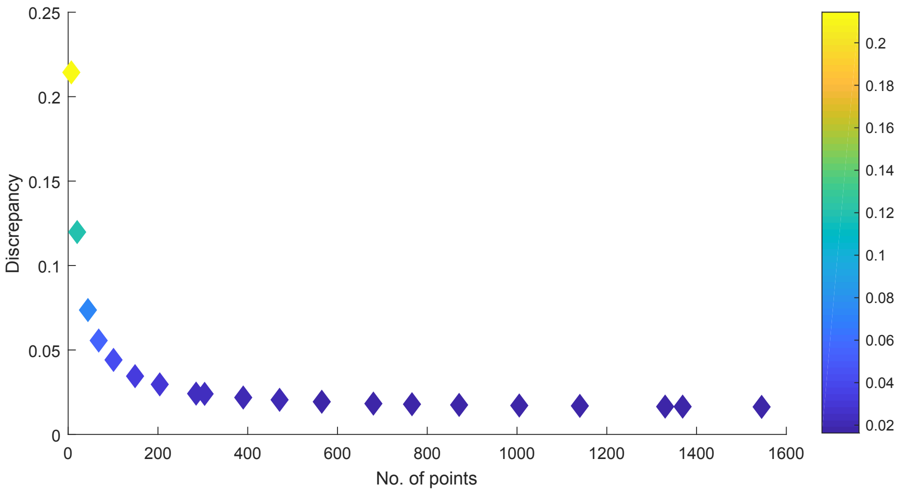
for $i, k \in \{1, 2, \ldots, N\}$ and $l_n \geq 0$, with the pseudodifferential operator $\mathcal{A} = \mathbb{A}_{\mathrm{X}}^{\frac{1}{2},\frac{3}{4}}$ and corresponding eigenvalues

$$A_{m,n} = \left(\mathbb{A}_{\mathrm{X}}^{\frac{1}{2},\frac{3}{4}}\right)^{\wedge}(m, n).$$

For type I, we use the representation (3.2) and representation (2.30) for type II to compute the kernel h. Note that we truncate the infinite sums in (3.4) up to degrees $\mathcal{M}$ and $\mathcal{N}$. Similar to the previous section, we take $\mathcal{M} = 50$, $\mathcal{N} = 50$ and $l_n = n$ for the case of type I and for type II, we choose $\mathcal{M} = 100$. Next, we use the *linsolve* command of matlab to solve the system (2.22) and consequently, find the unknowns α_i and λ. Having the value of λ, with the help of Theorem 2.3.3, we compute the weighted discrepancies with optimum weights α_i.



(a)



(b)

Figure 3.10: The behaviour of the weighted discrepancies with increasing number of points for the modified simple lattice corresponding to the orthonormal basis system of type I is shown in (a) and for type II in (b). The colourbar represents the values of the discrepancies.

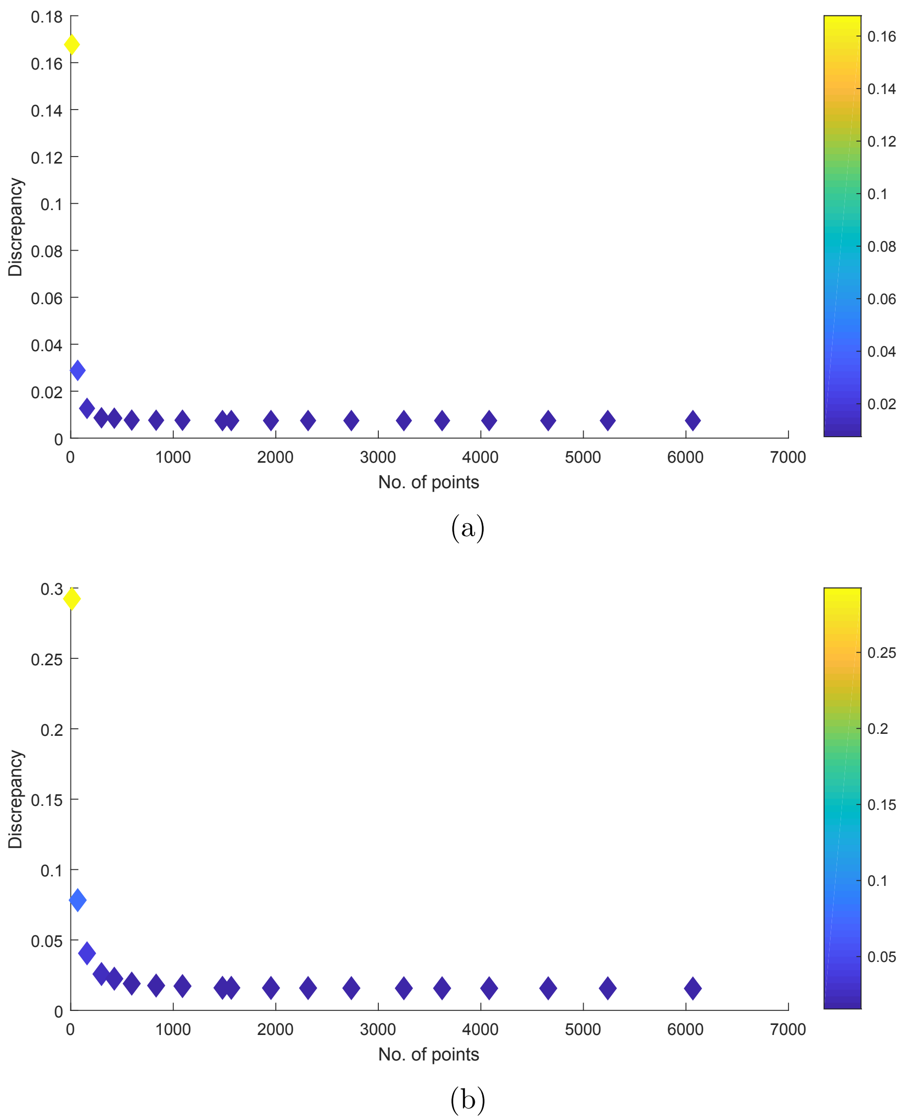
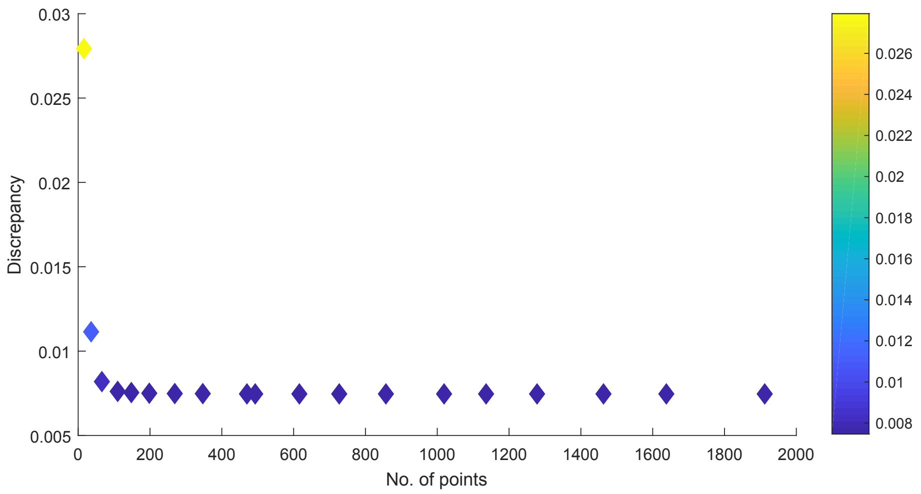
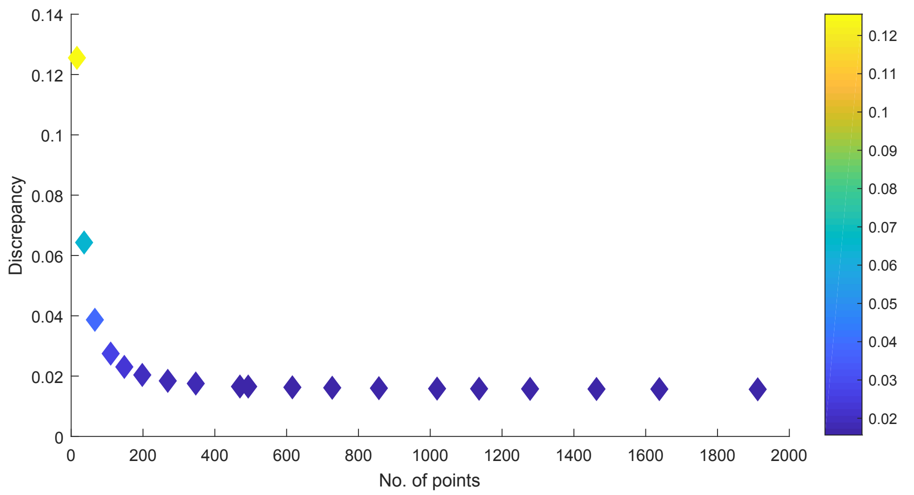


Figure 3.11: The behaviour of the weighted discrepancies with increasing number of points for the modified improved lattice corresponding to the orthonormal basis system of type I is shown in (a) and for type II in (b). The colourbar represents the values of the discrepancies.

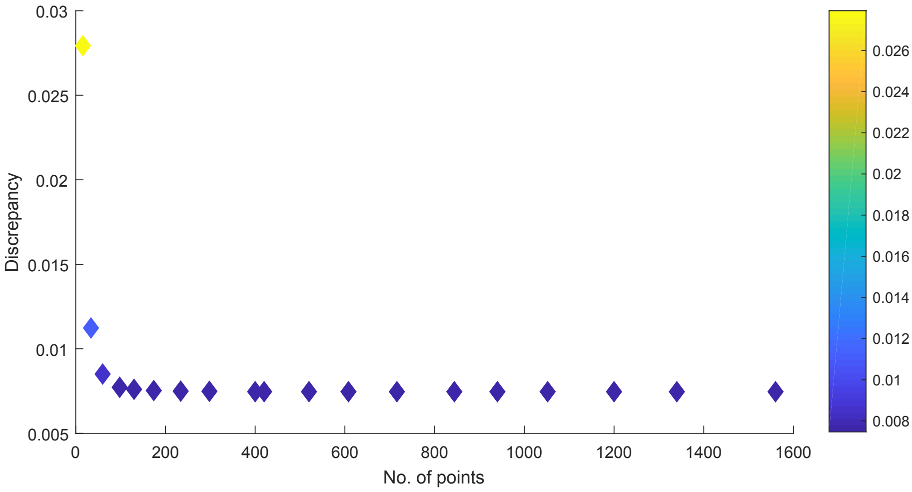


(a)

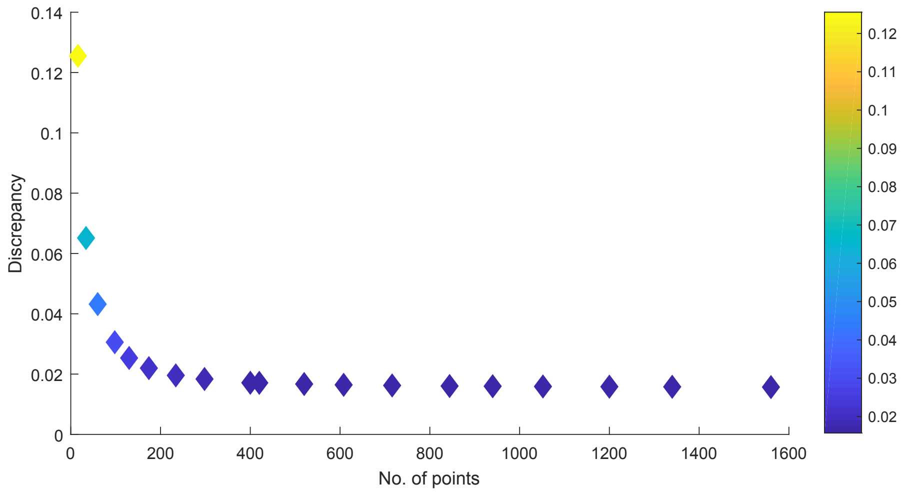


(b)

Figure 3.12: The behaviour of the weighted discrepancies with increasing number of points for the modified Reuter grid corresponding to the orthonormal basis system of type I is shown in (a) and for type II in (b). The colourbar represents the values of the discrepancies.



(a)



(b)

Figure 3.13: The behaviour of the weighted discrepancies with increasing number of points for the modified Freeden grid corresponding to the orthonormal basis system of type I is shown in (a) and for type II in (b). The colourbar represents the values of the discrepancies.

It appears from the plots that although the discrepancy estimates stagnate for large grids, the results are better than the previous case. The discrepancies behave more decently in this case and as the weights are chosen in order to minimize the discrepancy, the weighted case gives lower discrepancies (especially, for the case of type I) in comparison to the previous scenario.

Chapter 4

Lower Discrepancy Point Grids

In this chapter, we focus on finding lower discrepancy point grids along with the methods that minimize the discrepancy. We try different methods in order to find the algorithms which are further able to improve the existing grids from the previous chapter. In the following, the discrepancies are computed using equation (3.3) for the system of type I and (2.30) for type II with $p = \frac{1}{2}$, $q = \frac{3}{4}$ and weights $\alpha_i = \alpha_k = \frac{1}{N}$. Also, we truncate the infinite sums in these equations, as in Chapter 3. In the following, we denote a point grid by $X := (x_1, x_2, \ldots, x_N)$ and its $\imath$-th iteration by $X_\imath := (x_1^{(\imath)}, x_2^{(\imath)}, \ldots, x_N^{(\imath)})$.

4.1 Algorithms for the Point Grids

In order to have the point grids with lower value of discrepancies, we develop some algorithms. These methods require a starting grid which is then improved through a process. The algorithm stops after a given number of iterations or after satisfying a predefined stopping criterion. It is obvious that a good starting grid ensures a better resulting grid. This section gives a description of these methods and a graphical comparison between the discrepancies for the starting grid and the grid obtained after applying the algorithm.

1. Algorithm 1

    - Take a point grid X on the ball as a starting grid.
    - Calculate the neighbourhood distances of all the points.
    - Find the maximum neighbourhood distance M.
    - Take average of every two points having distance M.

- Create a new grid by excluding the points with distance M and including the average values.

As an example, we take the modified Reuter grid (see Section 3.1) as a starting grid in the algorithm. As mentioned above, it is an iterative process. The process stops, when the new maximum neighbourhood distance, say M_1 between the points on the ball is less than or equal to half of the previous distance M. We can deduce from the comparsion in Figure 4.1 that this method improves the initial grid and yields a grid with finer discrepancy estimates.

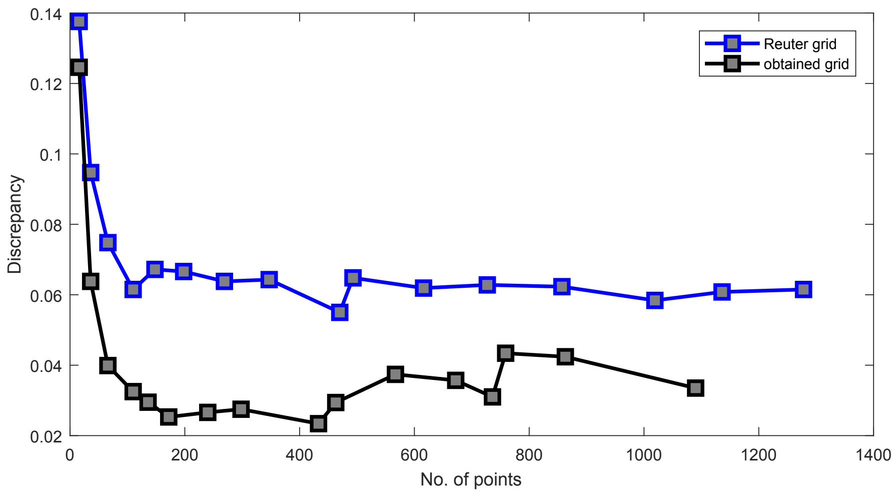


Figure 4.1: The plot shows the comparison of the discrepancy estimates computed for the modified Reuter grid with the estimates computed for the grid obtained from Algorithm 1.

2. Algorithm 2

   - Take a point grid X on the ball as a starting grid and a uniform grid $\{\eta^n\}_{n=1,2,\ldots,N}$ on the sphere as a helping grid.
   - Generate a random permutation $\{\eta^{P(n)}\}_{n=1,2,\ldots,N}$ of the grid on the sphere.
   - Generate random values $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_N$ for new lengths.
   - Create a new grid by setting $x_n^{(\imath+1)} = x_n^{(\imath)} + \varepsilon_n \cdot \eta^{P(n)}$.

We experiment with two grids in this case. We again choose the modified Reuter grid as the starting grid. In addition, we choose the Hammersley system ([24]) as a helping grid in the Figure 4.2a and the

Reuter grid on the sphere in Figure 4.2b. We generate the random permutations $\eta^{P(n)}$ of the helping grid by using the *randperm* command of Matlab and the lengths ε_n using the *rand* command of Matlab. Further, we exclude the points of the resulting grid that are outside the ball, i.e. points having norm greater than 1. This iterative method is stopped, when $D(X_{i+1}, \mathcal{A}) < 0.6 \cdot D(X_1, \mathcal{A})$. The plots in Figure 4.2 present the results obtained from the algorithm.

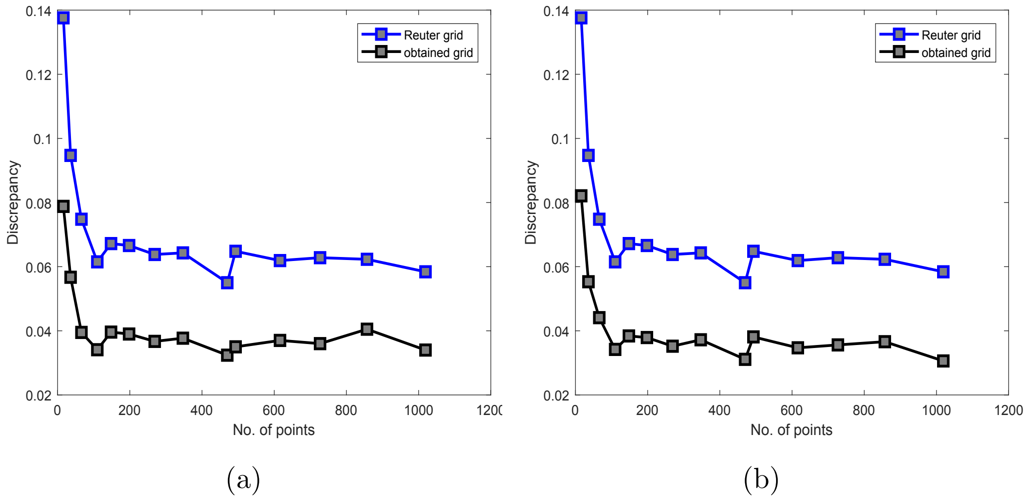


Figure 4.2: The plots show the comparisons of the discrepancy estimates between the starting grid and the resulting grid obtained from Algorithm 2 for two cases, that are: the modified Reuter grid with the Hammersley system in Subfigure (a) and the modified Reuter grid with the Reuter grid in Subfigure (b).

3. Algorithm 3

   - Take a point grid X on the ball as a starting grid.
   - Generate random angles of the size of the point grid.
   - Create a rotation matrix with these angles.
   - Create a new grid by rotating the starting grid using the rotation matrix.

In this algorithm, we took again the modified Reuter grid as the starting point. We choose the random angles with the *randn* command of matlab. For creating the rotation matrix, we use the command *make-hgtform* from matlab. Algorithm 3 stops, when it attains a predefined number of iterations. In this example, we choose a maximum number of iterations $\imath = 1000$. Figure 4.3 shows the behaviour of the point grid obtained from this algorithm as compared to the initial grid. As we can see from the graphical presentation, apart from some initial discrepancy values, the method does not improve the results.

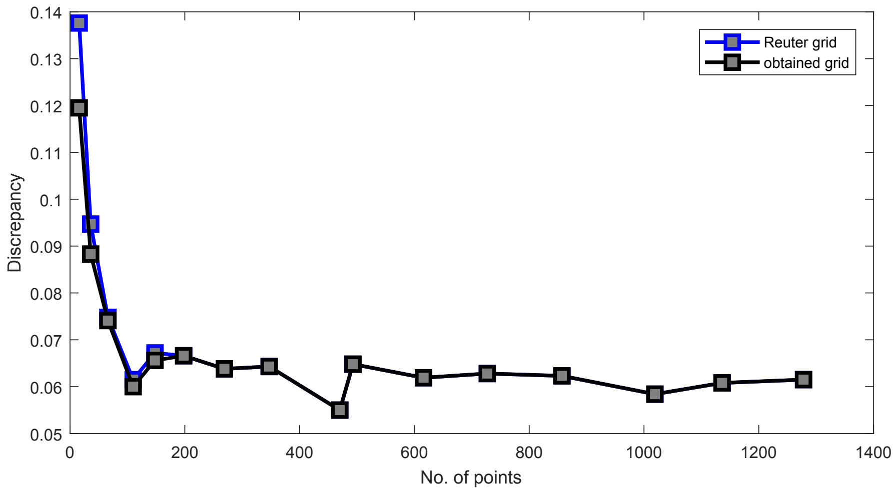


Figure 4.3: The plot shows a comparison of the results computed for the modified Reuter grid and the grid obtained from Algorithm 3.

4.2 BFGS Method

The Broyden-Fletcher-Goldfarb-Shanno (BFGS) method is a commonly used Quasi-Newton optimization procedure. In a general Quasi-Newton optimization technique, one requires the gradient $\nabla f_\imath := \nabla f(X_\imath)$ of the objective function f, a suitable point $X_\imath$ to start with and the Hessian matrix $B_\imath$. Then one obtains a search direction $p_\imath$, such that

$$B_\imath p_\imath = -\nabla f_\imath, \quad \imath \in \mathbb{N}_0. \tag{4.1}$$

This search direction is then followed to get a new point, i.e.

$$X_{\imath+1} = X_\imath + \gamma_\imath p_\imath, \tag{4.2}$$

where $\gamma_\imath$ is the suitable step size which is obtained by using a line search technique. Among other Quasi-Newton optimization procedures, the BFGS technique is very effective in the sense that it requires the approximation to

the Hessian matrix and updates it through each iteration instead of computing the exact Hessian each time.
Since our interest lies in acquiring low-discrepancy point grids, we use this method to minimize the nonlinear function (i.e. the discrepancy formula)

$$f_{\mathrm{obj,X}} = D^2\left(\omega_N, \mathbb{A}_{\mathrm{X}}^{\frac{1}{2},\frac{3}{4}}\right), \tag{4.3}$$

where for X = I with $l_n = n$, we have

$$f_{\mathrm{obj,I}} = \frac{1}{4\pi N^2}\left[\sum_{i,k=1}^{N}\sum_{m=0}^{\mathcal{M}}\sum_{n=0}^{\mathcal{N}} \varrho_{m,n} P_m^{(0,n+\frac{1}{2})}(2|x_i|^2-1) P_m^{(0,n+\frac{1}{2})}(2|x_k|^2-1)\right.$$
$$\left. \times\ (|x_i||x_k|)^n\, P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\right] - \frac{2}{9\pi}, \tag{4.4}$$

(see (3.3)) with

$$\varrho_{m,n} = \frac{(2n+1)(4m+2n+3)}{\left(\left(\mathbb{A}_{\mathrm{I}}^{\frac{1}{2},\frac{3}{4}}\right)^{\wedge}(m,n)\right)^2}$$
$$= \begin{cases} \frac{8}{(4m+3)^2}, & n=0,\ m\in\mathbb{N}_0 \\ \frac{8}{(4m+2n+3)^2 n(n+1)}, & n\in\mathbb{N},\ m\in\mathbb{N}_0, \end{cases}$$

and for X = II (see (2.30)),

$$f_{\mathrm{obj,II}} = \frac{2}{\pi N^2}\left[\sum_{i,k=1}^{N}\sum_{m=0}^{\mathcal{M}} \frac{2}{(2m+3)^2} P_m^{(0,2)}(2|x_i|-1) P_m^{(0,2)}(2|x_k|-1)\right.$$
$$\left. \times\left(1-\ln\left(1+\sqrt{\frac{1-\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}}{2}}\right)\right)\right] - \frac{2}{9\pi}. \tag{4.5}$$

In addition, we require the gradient of our objective function $f_{\mathrm{obj,X}}$. We note that for X = II, the objective function $f_{\mathrm{obj,II}}$ is not differentiable for all the points in the grid. Consequently, we are unable to use the BFGS method for type II with this particular representation. For this reason, we choose new values for the parameters p and q with $\alpha_i = \frac{1}{N}$ in (2.28). We use operator $\mathbb{A}_{\mathrm{II}}^{p,q}$ with $p = 1$ and $q = 1$ in (2.28) to get the objective function $f_{\mathrm{obj,II}}$ as

$$f_{\mathrm{obj,II}} = \frac{4}{\pi N^2}\left[\sum_{i,k=1}^{N}\sum_{m=0}^{\mathcal{M}} \frac{1}{(2m+3)^3} P_m^{(0,2)}(2|x_i|-1) P_m^{(0,2)}(2|x_k|-1)\right.$$
$$\left. \times\left(1+\sum_{n=1}^{\mathcal{N}}\frac{1}{(2n+1)n^2(n+1)^2} P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\right)\right] - \frac{4}{27\pi}. \tag{4.6}$$

Now, for finding the gradients of our objective functions, we need the gradients for Jacobi and Legendre polynomials. According to Theorem 1.2.8, we have

$$\begin{aligned}\nabla_{x_t} P_m^{(0,n+\frac{1}{2})}(2|x_i|^2-1) &= \frac{\Gamma(n+m+5/2)}{2\,\Gamma(n+m+3/2)}\, P_{m-1}^{(1,n+\frac{3}{2})}(2|x_i|^2-1)\, 4\, x_i^{\mathrm{T}}\, \nabla_{x_t} x_i \\ &= 2\left(n+m+\frac{3}{2}\right) P_{m-1}^{(1,n+\frac{3}{2})}(2|x_i|^2-1)\, x_i^{\mathrm{T}}\, \nabla_{x_t} x_i, \quad (4.7)\end{aligned}$$

where $\nabla_{x_t} x_i = \delta_{it} I$ and $t = 1, 2, \dots, N$ and

$$\begin{aligned}\nabla_{x_t} P_m^{(0,2)}(2|x_i|-1) &= \frac{\Gamma(m+4)}{2\,\Gamma(m+3)}\, P_{m-1}^{(1,3)}(2|x_i|-1)\, 2\left(\frac{x_i}{|x_i|}\right)^{\mathrm{T}} \nabla_{x_t} x_i \\ &= (m+3) P_{m-1}^{(1,3)}(2|x_i|-1)\left(\frac{x_i}{|x_i|}\right)^{\mathrm{T}} \nabla_{x_t} x_i. \qquad (4.8)\end{aligned}$$

For the Legendre polynomials, (1.36) yields

$$P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right) = C_n^{1/2}\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right).$$

Now, with the help of Theorem 1.1.2, Theorem 1.2.9 and the formula for surface gradient

$$\nabla_\xi^* F(\xi\cdot\eta) = F'(\xi\cdot\eta)[\eta - (\xi\cdot\eta)\xi] \qquad (4.9)$$

from [47], we obtain

$$\begin{aligned}&\nabla_{x_t} P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right) \\ &= \nabla_{x_t} C_n^{1/2}\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right) \\ &= \frac{1}{|x_t|} C_{n-1}^{3/2}\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right) \nabla^*_{\frac{x_t}{|x_t|}}\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right) \\ &= \frac{1}{|x_t|} C_{n-1}^{3/2}\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\left[\delta_{it}\left(\frac{x_k}{|x_k|} - \left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\frac{x_i}{|x_i|}\right)\right. \\ &\quad \left. + \delta_{kt}\left(\frac{x_i}{|x_i|} - \left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\frac{x_k}{|x_k|}\right)\right]. \qquad (4.10)\end{aligned}$$

Furthermore, for the term $(|x_i||x_k|)^n$, we get

$$\nabla_{x_t}\left(|x_i||x_k|\right)^n = n\left(|x_i||x_k|\right)^{n-1}\left(|x_i|\left(\frac{x_k}{|x_k|}\right)^{\mathrm{T}} \nabla_{x_t} x_k + \left(\frac{x_i}{|x_i|}\right)^{\mathrm{T}} \nabla_{x_t} x_i |x_k|\right). \qquad (4.11)$$

Hence, all the above calculations and the product rule for gradients yield

$$
\begin{aligned}
\nabla_{x_t} f_{\mathrm{obj,I}} = \frac{1}{4\pi N^2} \sum_{i,k=1}^{N} \Bigg[\sum_{m=1}^{\mathcal{M}} \sum_{n=0}^{\mathcal{N}} 2\varrho_{m,n} \left(n+m+\frac{3}{2}\right) \Big(P_{m-1}^{(1,n+\frac{3}{2})}(2|x_i|^2-1) \\
\times x_i^{\mathrm{T}} \nabla_t x_i P_m^{(0,n+\frac{1}{2})}(2|x_k|^2-1) + P_{m-1}^{(1,n+\frac{3}{2})}(2|x_k|^2-1) x_k^{\mathrm{T}} \nabla_t x_k P_m^{(0,n+\frac{1}{2})}(2|x_i|^2-1) \Big) \\
\times \left(|x_i||x_k|\right)^n P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right) + \sum_{m=0}^{\mathcal{M}} \sum_{n=1}^{\mathcal{N}} \varrho_{m,n} n \left(|x_i||x_k|\right)^{n-1} P_m^{(0,n+\frac{1}{2})}(2|x_i|^2-1) \\
\times P_m^{(0,n+\frac{1}{2})}(2|x_k|^2-1) \left(|x_i| \left(\frac{x_k}{|x_k|}\right)^{\mathrm{T}} \nabla_{x_t} x_k + \left(\frac{x_i}{|x_i|}\right)^{\mathrm{T}} \nabla_{x_t} x_i |x_k| \right) \\
\times P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right) + \sum_{m=0}^{\mathcal{M}} \sum_{n=1}^{\mathcal{N}} \varrho_{m,n} P_m^{(0,n+\frac{1}{2})}(2|x_i|^2-1) P_m^{(0,n+\frac{1}{2})}(2|x_k|^2-1) \\
\times \left(\delta_{it} \left(\frac{x_k}{|x_k|} - \left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\frac{x_i}{|x_i|} \right) + \delta_{kt} \left(\frac{x_i}{|x_i|} - \left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\frac{x_k}{|x_k|} \right) \right) \\
\times \frac{\left(|x_i||x_k|\right)^n}{|x_t|} C_{n-1}^{3/2}\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right) \Bigg]. \quad (4.12)
\end{aligned}
$$

Consequently, we get

$$
\begin{aligned}
&\nabla_{x_t} f_{\mathrm{obj,I}} \\
&= \frac{1}{2\pi N^2} \sum_{i=1}^{N} \Bigg[\sum_{m=1}^{\mathcal{M}} \sum_{n=0}^{\mathcal{N}} 2\varrho_{m,n} \left(n+m+\frac{3}{2}\right) x_t P_{m-1}^{(1,n+\frac{3}{2})}(2|x_t|^2-1) \\
&\times P_m^{(0,n+\frac{1}{2})}(2|x_i|^2-1) \left(|x_i||x_t|\right)^n P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_t}{|x_t|}\right) + \sum_{m=0}^{\mathcal{M}} \sum_{n=1}^{\mathcal{N}} \varrho_{m,n} n \left(|x_i||x_t|\right)^{n-1} \\
&\times P_m^{(0,n+\frac{1}{2})}(2|x_i|^2-1) P_m^{(0,n+\frac{1}{2})}(2|x_t|^2-1) P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_t}{|x_t|}\right) |x_i| \frac{x_t}{|x_t|} \\
&+ \sum_{m=0}^{\mathcal{M}} \sum_{n=1}^{\mathcal{N}} \varrho_{m,n} \frac{\left(|x_i||x_t|\right)^n}{|x_t|} P_m^{(0,n+\frac{1}{2})}(2|x_i|^2-1) P_m^{(0,n+\frac{1}{2})}(2|x_t|^2-1) \\
&\times \left(\frac{x_i}{|x_i|} - \left(\frac{x_i}{|x_i|}\cdot\frac{x_t}{|x_t|}\right)\frac{x_t}{|x_t|} \right) C_{n-1}^{3/2}\left(\frac{x_i}{|x_i|}\cdot\frac{x_t}{|x_t|}\right) \Bigg], \quad (4.13)
\end{aligned}
$$

for X = I. Analogously, for X = II, we obtain

$$\begin{aligned}
&\nabla_{x_t} f_{\mathrm{obj,II}} \\
&= \frac{4}{\pi N^2} \sum_{i,k=1}^{N} \Bigg[\sum_{m=1}^{\mathcal{M}} \frac{(m+3)}{(2m+3)^3} \Bigg(P_m^{(0,2)}(2|x_i|-1) P_{m-1}^{(1,3)}(2|x_k|-1) \left(\frac{x_k}{|x_k|}\right)^{\mathrm{T}} \nabla_{x_t} x_k \\
&\qquad + P_m^{(0,2)}(2|x_k|-1) P_{m-1}^{(1,3)}(2|x_i|-1) \left(\frac{x_i}{|x_i|}\right)^{\mathrm{T}} \nabla_{x_t} x_i \Bigg) \\
&\qquad \times \left(1 + \sum_{n=1}^{\mathcal{N}} \frac{1}{(2n+1)n^2(n+1)^2} P_n\left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right)\right) \\
&\qquad + \left(\sum_{m=0}^{\mathcal{M}} \frac{1}{(2m+3)^3} P_m^{(0,2)}(2|x_i|-1) P_m^{(0,2)}(2|x_k|-1)\right) \\
&\qquad \times \left(\sum_{n=1}^{\mathcal{N}} \frac{1}{(2n+1)n^2(n+1)^2} \frac{1}{|x_t|} C_{n-1}^{3/2}\left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right)\right) \\
&\times \left(\delta_{it}\left(\frac{x_k}{|x_k|} - \left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right)\frac{x_i}{|x_i|}\right) + \delta_{kt}\left(\frac{x_i}{|x_i|} - \left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right)\frac{x_k}{|x_k|}\right)\right)\Bigg],
\end{aligned}$$

which finally yields

$$\begin{aligned}
\nabla_{x_t} f_{\mathrm{obj,II}} &= \frac{4}{\pi N^2} \sum_{i=1}^{N} \Bigg[\sum_{m=1}^{\mathcal{M}} \frac{2(m+3)}{(2m+3)^3} P_m^{(0,2)}(2|x_i|-1) P_{m-1}^{(1,3)}(2|x_t|-1) \frac{x_t}{|x_t|} \\
&\qquad \times \left(1 + \sum_{n=1}^{\mathcal{N}} \frac{1}{(2n+1)n^2(n+1)^2} P_n\left(\frac{x_i}{|x_i|} \cdot \frac{x_t}{|x_t|}\right)\right) \\
&\quad + \left(\sum_{m=0}^{\mathcal{M}} \frac{1}{(2m+3)^3} P_m^{(0,2)}(2|x_i|-1) P_m^{(0,2)}(2|x_t|-1)\right) \\
\times \sum_{n=1}^{\mathcal{N}} &\frac{2}{(2n+1)n^2(n+1)^2} C_{n-1}^{3/2}\left(\frac{x_i}{|x_i|} \cdot \frac{x_t}{|x_t|}\right) \frac{1}{|x_t|}\left(\frac{x_i}{|x_i|} - \left(\frac{x_i}{|x_i|} \cdot \frac{x_t}{|x_t|}\right)\frac{x_t}{|x_t|}\right)\Bigg].
\end{aligned} \tag{4.14}$$

Having the gradient of our objective functions, we further need a method to update the Hessian and a line search algorithm. We experimented with different methods in order to find out the one which works best in our case. We tested two other updates, the damped BFGS update and the LDL^{T} factors ([28, 29, 54]) for updating the Hessian approximation matrix, along with the usual BFGS update. Both of these updates are closely related to the BFGS update. Furthermore, we use different line search methods (see, for example [29, 54]). That are:

1. $\gamma_\imath = \frac{9}{\imath}$,
2. $\gamma_\imath = \frac{9}{\sqrt{\imath}}$,
3. Wolfe line search condition, i.e. $\gamma_\imath$ has to satisfy the following conditions:

$$f(X_\imath + \gamma_\imath p_\imath) \leq f(X_\imath) + c_1 \gamma_\imath \nabla f_\imath^{\mathrm{T}} p_\imath,$$
$$\nabla f(X_\imath + \gamma_\imath p_\imath)^{\mathrm{T}} p_\imath \geq c_2 \nabla f_\imath^{\mathrm{T}} p_\imath,$$

with $0 < c_1 < c_2 < 1$. For our tests, we choose $c_1 = 10^{-4}$ and $c_2 = 0.9$.

4. Backtracking line search, i.e. $\gamma_\imath$ has to satisfy the following condition:

$$f(x_\imath + \gamma_\imath p_\imath) \leq f(x_\imath) + c \gamma_\imath \nabla f_\imath^{\mathrm{T}} p_\imath,$$

with $0 < c < 1$. We choose $c = 0.01$ for our experiments. This condition also appears in the Wolfe line search and is known as sufficient decrease condition. Wolfe line search together with the additional second condition is considered to be stronger than the backtracking line search ([54]).

It is observed that the difference in the line search methods also affects the outcomes and the rate of convergence. We use the modified Reuter grid of 616 points as a starting grid in the following tests. The stopping criteria for the algorithm is set as follows

$$\|\nabla f_\imath\| < \epsilon, \quad \epsilon > 0.$$

We choose $\epsilon = 10^{-8}$ for $f_{\text{obj,I}}$ and $\epsilon = 10^{-4}$ for $f_{\text{obj,II}}$. If the algorithm does not satisfy the tolerance level ϵ, it is stopped after reaching the predetermined number of iterations. In our tests, we take the maximum number of iterations $\imath = 500$ and for the computation of $f_{\text{obj,X}}$ and its gradient, we choose $\mathcal{M} = 10$ and $\mathcal{N} = 10$. Figures 4.4 to 4.9 show the plots of the results obtained, using the above mentioned techniques.

1. **BFGS Update.**
   The updating formula for the Hessian approximation $B_\imath$ is given as

$$B_{\imath+1} := B_\imath - \frac{B_\imath s_\imath s_\imath^{\mathrm{T}} B_\imath}{s_\imath^{\mathrm{T}} B_\imath s_\imath} + \frac{y_\imath y_\imath^{\mathrm{T}}}{y_\imath^{\mathrm{T}} s_\imath}, \tag{4.15}$$

where

$$s_\imath := X_{\imath+1} - X_\imath = \gamma_\imath p_\imath$$

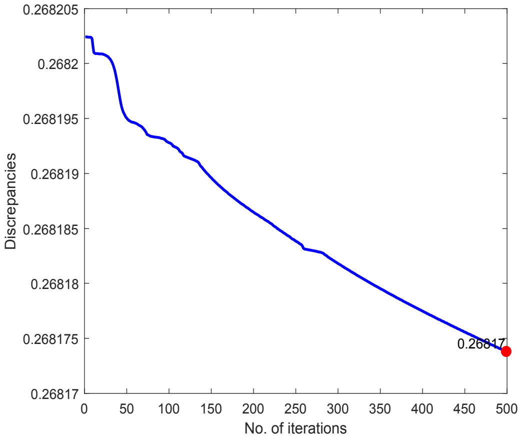
and

$$y_\imath := \nabla f_{\imath+1} - \nabla f_\imath.$$

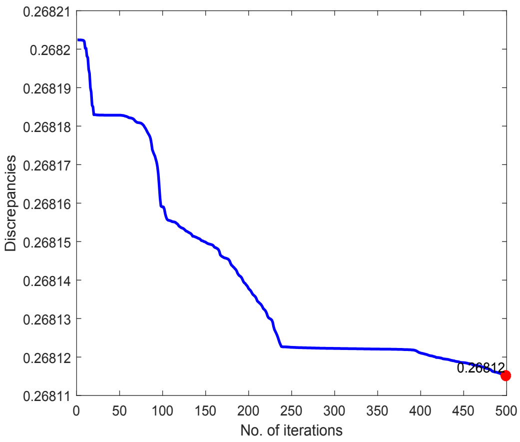
Note that the curvature condition

$$s_\imath^{\mathrm{T}} y_\imath > 0 \tag{4.16}$$

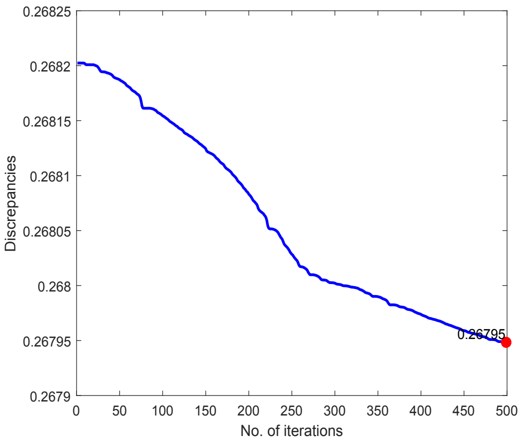
guarantees that the Hessian approximation update at each iteration is positive definite, which is an important prospect for the convergence of the function to a minimum value ([54]). The update (4.15) along with only an appropriate line search method can assure the attainment of this condition. Figures 4.4 and 4.5 show the results of the BFGS method using the BFGS update, i.e. (4.15).



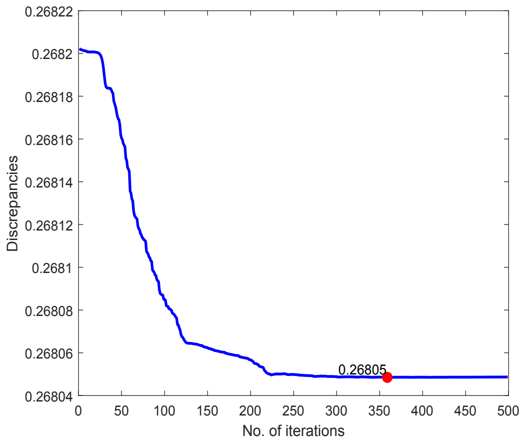
(a) $\gamma_\imath = \frac{9}{\imath}$



(b) $\gamma_\imath = \frac{9}{\sqrt{\imath}}$

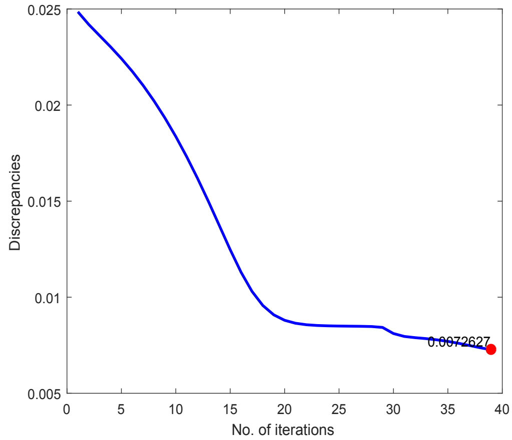


(c) Backtracking line search

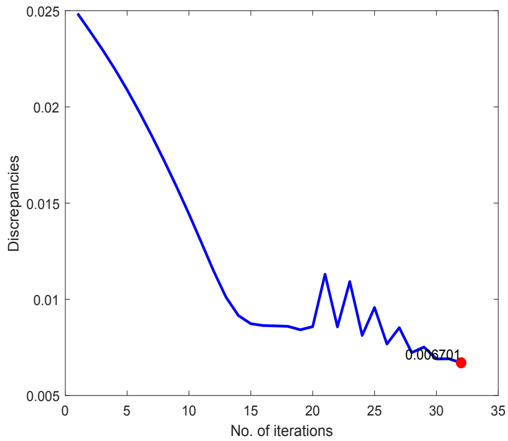


(d) Wolfe line search

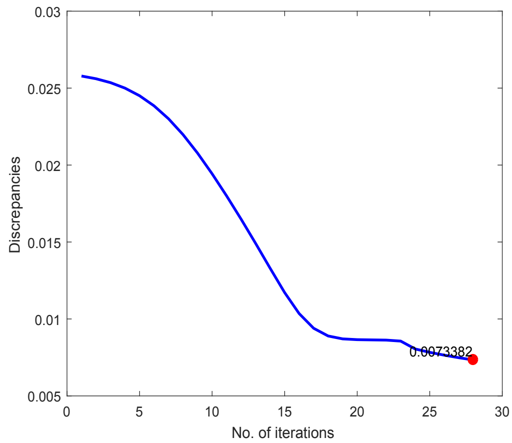
Figure 4.4: The plots show the behaviour of the discrepancies for the orthonormal system of type I using the BFGS update (4.15) corresponding to the number of iterations. The red point represents the minimum value of discrepancy.



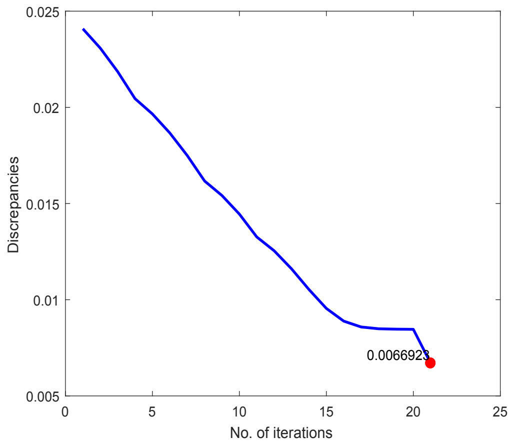
(a) $\gamma_\imath = \frac{9}{\imath}$



(b) $\gamma_\imath = \frac{9}{\sqrt{\imath}}$



(c) Backtracking line search



(d) Wolfe line search

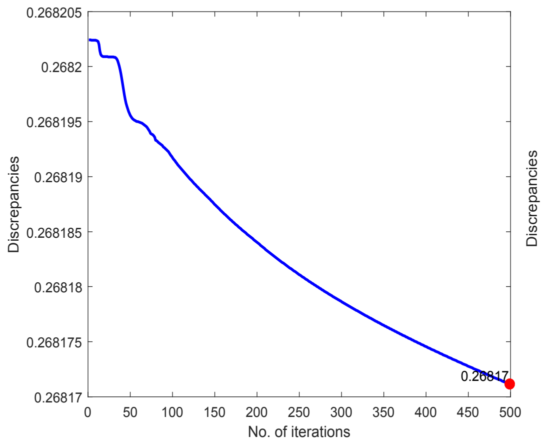
Figure 4.5: The plots show the behaviour of the discrepancies for the orthonormal system of type II using the BFGS update (4.15) corresponding to the number of iterations. The red point represents the minimum value of discrepancy.

2. **Damped BFGS Update.**
For $s_\imath := X_{\imath+1} - X_\imath := \gamma_\imath p_\imath$ and $r_\imath := \theta_\imath y_\imath + (1-\theta_\imath) B_\imath s_\imath$, the damped BFGS updating formula for the Hessian approximation B_i is given as:

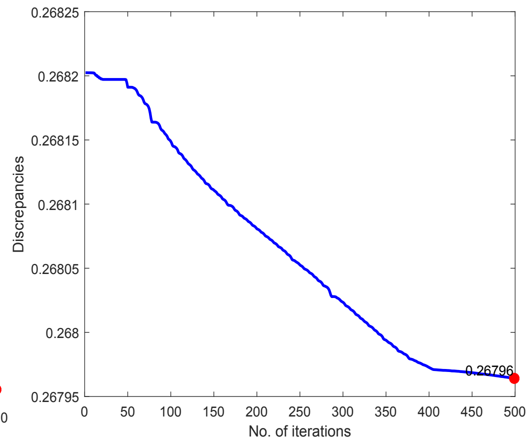
$$B_{\imath+1} := B_\imath - \frac{B_\imath s_\imath s_\imath^{\mathrm{T}} B_\imath}{s_\imath^{\mathrm{T}} B_\imath s_\imath} + \frac{r_\imath r_\imath^{\mathrm{T}}}{r_\imath^{\mathrm{T}} s_\imath}, \tag{4.17}$$

where $y_\imath := \nabla f_{\imath+1} - \nabla f_\imath$ and

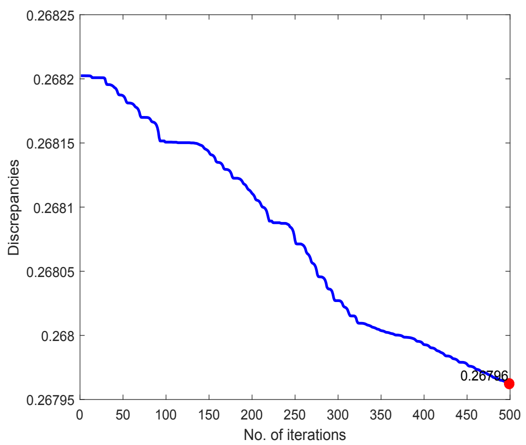
$$\theta_\imath := \begin{cases} 1, & s_\imath^{\mathrm{T}} y_\imath \geq 0.2 s_\imath^{\mathrm{T}} B_\imath s_\imath, \\ \frac{0.8 s_\imath^{\mathrm{T}} B_\imath s_\imath}{s_\imath^{\mathrm{T}} B_\imath s_\imath - s_\imath^{\mathrm{T}} y_\imath}, & s_\imath^{\mathrm{T}} y_\imath < 0.2 s_\imath^{\mathrm{T}} B_\imath s_\imath. \end{cases}$$



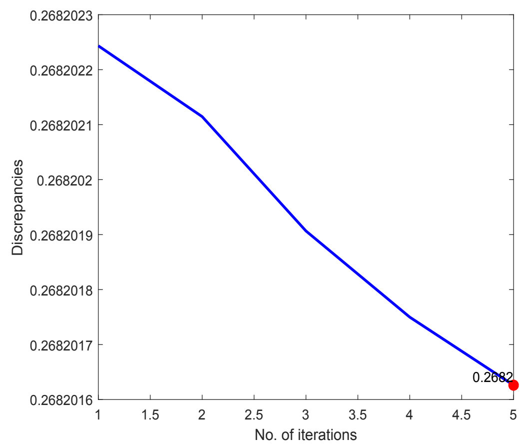
(a) $\gamma_\imath = \frac{9}{\imath}$



(b) $\gamma_\imath = \frac{9}{\sqrt{\imath}}$



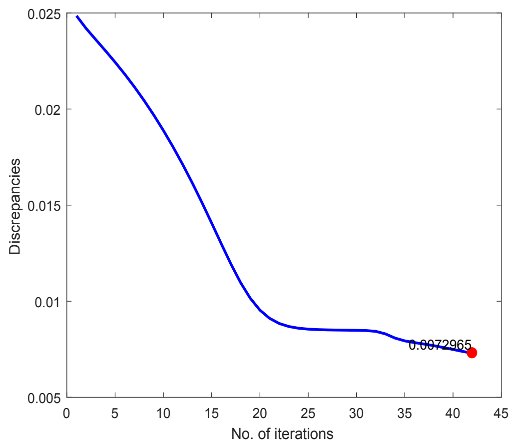
(c) Backtracking line search



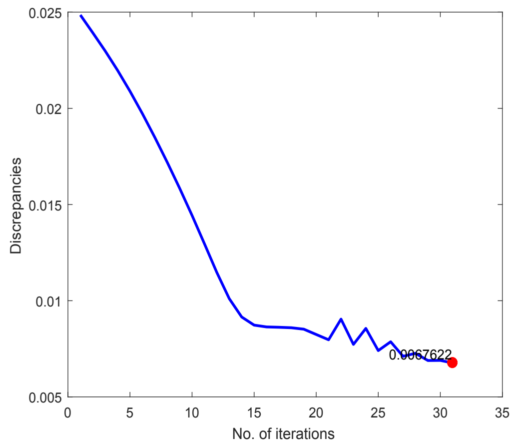
(d) Wolfe line search

Figure 4.6: The plots show the behaviour of the discrepancies for the orthonormal basis system of type I using the damped BFGS update (4.17) corresponding to the number of iterations. The red point represents the minimum value of discrepancy.

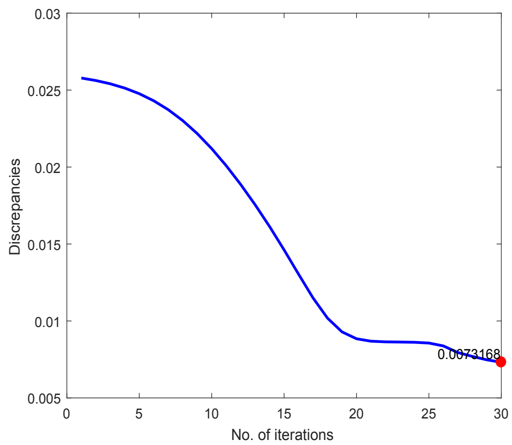
Note that (4.17) is the same as (4.15) for $r_\imath = y_\imath$. This update ensures that the curvature condition (4.16) holds, which consequently guarantees the positive definiteness of the Hessian approximation matrix $B_\imath$. The results for the BFGS method using the damped BFGS update are shown in Figures 4.6 and 4.7.



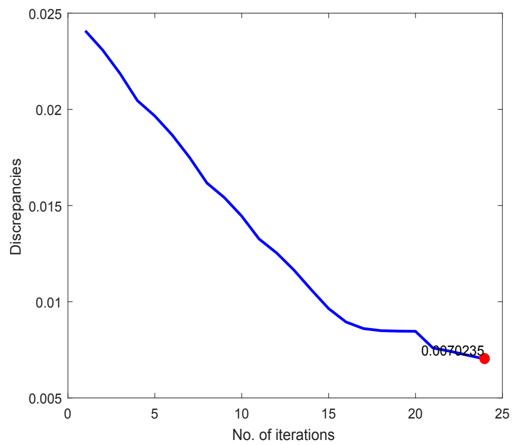
(a) $\gamma_\imath = \frac{9}{\imath}$



(b) $\gamma_\imath = \frac{9}{\sqrt{\imath}}$



(c) Backtracking line search



(d) Wolfe line search

Figure 4.7: The plots show the behaviour of the discrepancies for the orthonormal basis system of type II using the damped BFGS update (4.17) corresponding to the number of iterations. The red point represents the minimum value of discrepancy.

3. LDL^{T} **factors update.**
   Another effective method to update B_i, is to use the Cholesky factor-

ization LDL^{T} of the Hessian instead of the Hessian itself. With

$$B_0 = LDL^{\mathrm{T}},$$

the update is given as

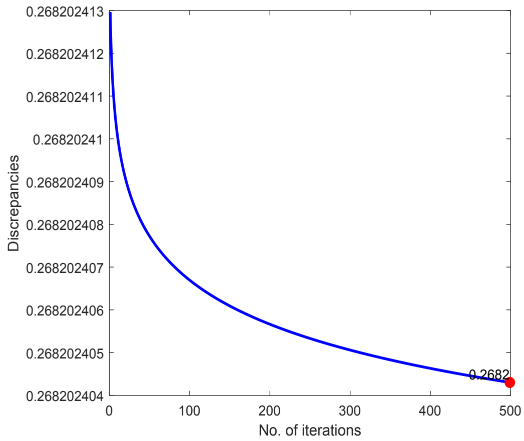
$$B_{\imath+1} := B_\imath + \beta z z^{\mathrm{T}},$$

where z is a vector such that zz^{T} is a one rank matrix and β is a constant. For $p = L^{-1}z$ we have

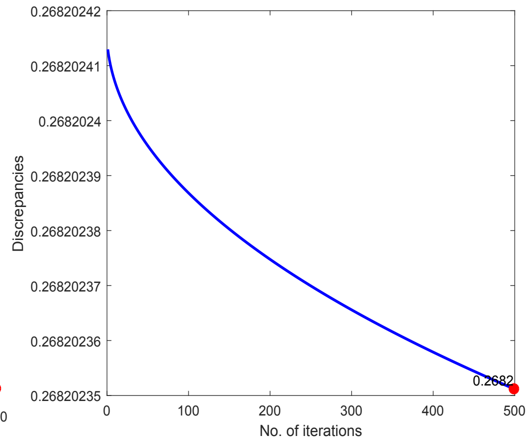
$$\begin{aligned} B_{\imath+1} = L_\imath D_\imath L_\imath^{\mathrm{T}} + \beta z z^{\mathrm{T}} &= L_\imath D_\imath L_\imath^{\mathrm{T}} + \beta (L_\imath L_\imath^{-1}) z z^{\mathrm{T}} (L_\imath^{-\mathrm{T}} L_\imath^{\mathrm{T}}) \\ &= L_\imath D_\imath L_\imath^{\mathrm{T}} + \beta L_\imath p p^{\mathrm{T}} L_\imath^{\mathrm{T}} \\ &= L_\imath (D_\imath + \beta p p^{\mathrm{T}}) L_\imath^{\mathrm{T}}. \end{aligned} \tag{4.18}$$

For the following tests, we choose $\beta = 1$ and $z = (0, \dots, 0, 1) \in \mathbb{R}^N$, N being the length of the grid X. The plots in Figures 4.8 and 4.9 show the results computed using the BFGS method with the LDL^{T} factors update.

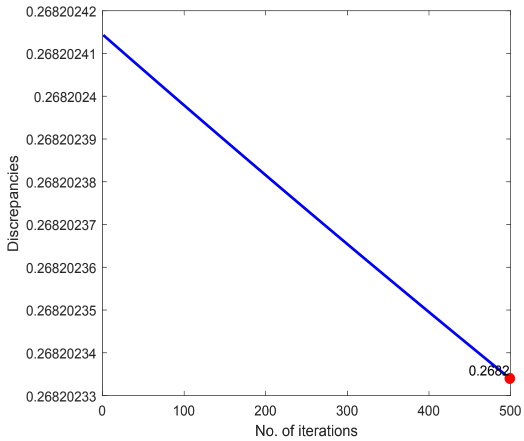
The Tables 4.1 and 4.2 combine the results for the orthonormal basis systems of type I and type II. The tables show a comparison between the applied methods. It is evident from the results that the convergence rate for the discrepancy of type I is very slow, while the BFGS method yields good results for type II. The different BFGS updates and line search techniques used here give different convergence rates and estimates of discrepancies. For example, for type I, the backtracking line search method gives better estimates both for the BFGS update and the damped BFGS update, whereas the Wolfe conditions require less number of iterations for the damped BFGS update and the LDL^{T} factors update. For type II, the Wolfe conditions as a line search technique give better results for a lower number of iterations in comparison to other methods for the case of the BFGS update, while for the case of the damped BFGS update the line search technique $\gamma_\imath = \frac{9}{\sqrt{\imath}}$ gives better results. When we look at the results for the LDL^{T} factors update, Wolfe conditions give the best outcome. Also, the overall comparison of the results show that the combination of LDL^{T} factors update with the Wolfe conditions gives better results for a lower number of iterations in comparison to the other methods.



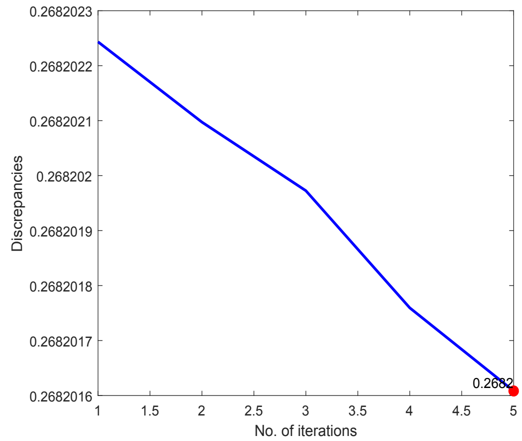
(a) $\gamma_\imath = \frac{9}{\imath}$



(b) $\gamma_\imath = \frac{9}{\sqrt{\imath}}$

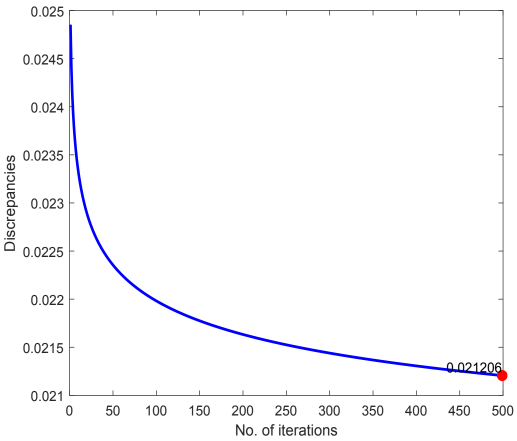


(c) Backtracking line search

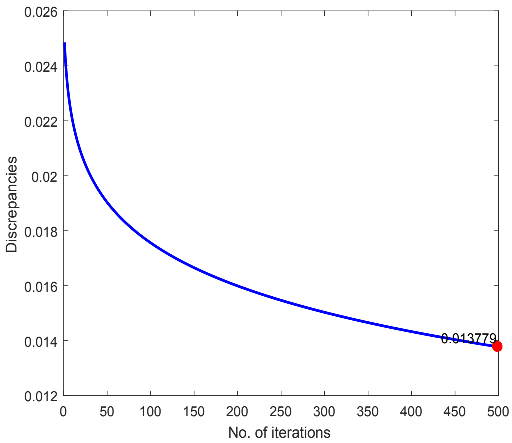


(d) Wolfe line search

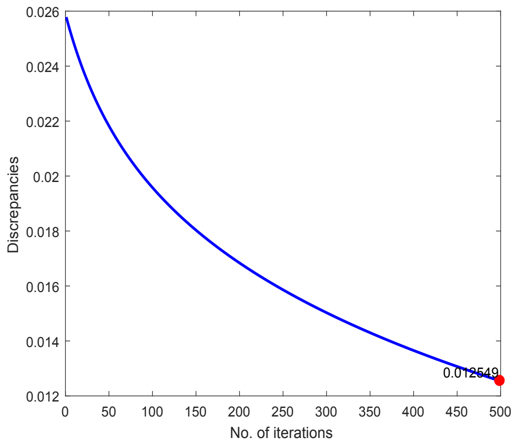
Figure 4.8: The plots show the behaviour of the discrepancies for the orthonormal basis system of type I using the LDL^{T} factors update (4.18) corresponding to the number of iterations. The red point represents the minimum value of discrepancy.



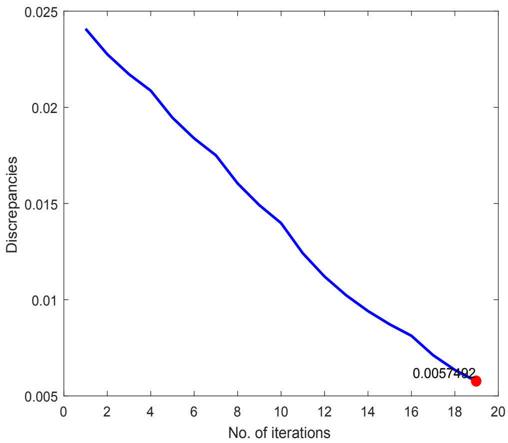
(a) $\gamma_\imath = \frac{9}{\imath}$



(b) $\gamma_\imath = \frac{9}{\sqrt{\imath}}$



(c) Backtracking line search



(d) Wolfe line search

Figure 4.9: The plots show the behaviour of the discrepancies for the orthonormal basis system of type II using the LDL^{T} factors update (4.18) corresponding to the number of iterations. The red point represents the minimum value of discrepancy.

Table 4.1

$\gamma_\imath$	$\frac{9}{\imath}$	$\frac{9}{\sqrt{\imath}}$	Wolfe line search	Backtracking line search
BFGS update	0.26817	0.26812	0.26805	0.26795
damped BFGS update	0.26817	0.26796	0.2682	0.26796
LDL^{T} factors update	0.2682	0.2682	0.2682	0.2682

The table shows the minimum values of discrepancies (type I), using the BFGS method with different updates and line search techniques.

Table 4.2

$\gamma_\imath$	$\frac{9}{\imath}$	$\frac{9}{\sqrt{\imath}}$	Wolfe line search	Backtracking line search
BFGS update	0.007262	0.006701	0.006692	0.007338
damped BFGS update	0.007296	0.006762	0.007023	0.007316
LDL^{T} factors update	0.028964	0.013779	0.005492	0.012549

The table shows the minimum values of discrepancies (type II), using the BFGS method with different updates and line search techniques.

Chapter 5

Statistical Computation

The generalized discrepancy (2.17), due to its structure, has some interesting statistical aspects depending on the specific point grid. In this chapter, we discuss some characteristics for the discrepancy using a sample $\mathcal{P}_N$ of N independent and identically distributed grid points on the ball $\mathcal{B}_R$.

5.1 Asymptotic Properties of Generalized Discrepancy

We assume that $\sigma(\cdot)$ is the measure defined on the ball $\mathcal{B}_R$ of radius R and $\sigma^*(\cdot)$ is the uniform probability measure, then $\sigma^*(\cdot) = \frac{\sigma(\cdot)}{\sigma(\mathcal{B}_R)} = \frac{3}{4\pi R^3}\sigma(\cdot)$, since $\sigma(\mathcal{B}_R) = \frac{4\pi}{3}R^3$. Then we have the variance and expectation of the orthonormal systems $G^{\mathrm{X}}_{m,n,j}$ as follows

$$\mathbb{V}\left(G^{\mathrm{X}}_{m,n,j}(x)\right) := \int_{\mathcal{B}_R} \left(G^{\mathrm{X}}_{m,n,j}(x)\right)^2 \mathrm{d}\sigma^*(x) = \frac{3}{4\pi R^3} \quad \text{for } (m,n,j) \neq (0,0,1); \; l_0 = 0 \quad (5.1)$$

and

$$\mathbb{E}\left(G^{\mathrm{X}}_{m,n,j}(x)\right) := \int_{\mathcal{B}_R} G^{\mathrm{X}}_{m,n,j}(x)\mathrm{d}\sigma^*(x) = 0 \quad \text{for } (m,n,j) \neq (0,0,1); \; l_0 = 0. \quad (5.2)$$

Note that we are working in a Sobolev space where $\left\langle F, G^{\mathrm{X}}_{m,n,j}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R)} = 0$ whenever $A_{m,n} = 0$ or $l_n < 0$ (see Definition 1.4.5). Hence, throughout this chapter $A_{m,n}$ is a non-vanishing sequence and $l_n \in \mathbb{R}^+_0$.

Theorem 5.1.1 *Let the sequence* $\{A_{m,n}\}_{(m,n)\neq(0,0)}$ *satisfy the summability conditions* (1.63) *and* (1.64) *for* X = I *and* X = II, *respectively. Then the series*

$$\sum_{1\leq i\neq k\leq N}\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}}\sum_{j=1}^{2n+1}\frac{1}{N^2}\frac{G^{\mathrm{X}}_{m,n,j}(x_i)G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}},\quad m,n\in\mathbb{N}_0 \tag{5.3}$$

converges uniformly with respect to x_i, x_k *and* N.

Proof: Considering first the orthonormal basis system $G^{\mathrm{I}}_{m,n,j}$ given by (1.50), we have

$$\begin{aligned}
&\sum_{1\leq i\neq k\leq N}\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}}\left|\sum_{j=1}^{2n+1}\frac{1}{N^2}\frac{G^{\mathrm{I}}_{m,n,j}(x_i)G^{\mathrm{I}}_{m,n,j}(x_k)}{A^2_{m,n}}\right|\\
&=\sum_{i\neq k}\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}}\left|\frac{1}{N^2}\frac{(2n+1)(4m+2l_n+3)}{4\pi R^3A^2_{m,n}}P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{|x_i|^2}{R^2}-1\right)\right.\\
&\qquad\left.\times P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{|x_k|^2}{R^2}-1\right)\left(\frac{|x_i||x_k|}{R^2}\right)^{l_n}P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\right|\\
&=\sum_{i\neq k}\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}}\frac{1}{N^2}\frac{(2n+1)(4m+2l_n+3)}{4\pi R^3A^2_{m,n}}\left|P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{|x_i|^2}{R^2}-1\right)\right|\\
&\qquad\times\left|P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{|x_k|^2}{R^2}-1\right)\right|\left|\left(\frac{|x_i||x_k|}{R^2}\right)^{l_n}\right|\left|P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\right|
\end{aligned}$$

The fact

$$\frac{|x_i||x_k|}{R^2}\leq 1 \tag{5.4}$$

and Theorem 1.2.10 for the absolute maximum of the Jacobi and the Legendre polynomials enable us to deduce the following:

$$\begin{aligned}
&\sum_{1\leq i\neq k\leq N}\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}}\left|\sum_{j=1}^{2n+1}\frac{1}{N^2}\frac{G^{\mathrm{I}}_{m,n,j}(x_i)G^{\mathrm{I}}_{m,n,j}(x_k)}{A^2_{m,n}}\right|\\
&\qquad\leq\sum_{i\neq k}\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}}\frac{1}{N^2}\frac{(2n+1)(4m+2l_n+3)}{4\pi R^3A^2_{m,n}}\binom{m+l_n+\frac{1}{2}}{m}^2.
\end{aligned}\tag{5.5}$$

Further, using the estimate (1.60) and the summability condition (1.63), we get

$$\begin{aligned}
&\sum_{1\le i\neq k\le N}\ \sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} \left| \sum_{j=1}^{2n+1} \frac{1}{N^2} \frac{G^{\mathrm{I}}_{m,n,j}(x_i)G^{\mathrm{I}}_{m,n,j}(x_k)}{A^2_{m,n}} \right| \\
&\le \frac{N(N-1)}{4\pi R^3 N^2} \left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} \frac{(2n+1)(4m+2l_n+3)}{A^2_{m,n}} \frac{(m+l_n+\frac{1}{2})^{2m}}{(m!\,)^2} \right) \\
&\le \underbrace{\left(1-\frac{1}{N}\right)}_{\le 1} \left(\frac{1}{4\pi R^3}\right) \underbrace{\left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} \frac{(2n+1)(4m+2l_n+3)}{A^2_{m,n}} \frac{(m+l_n+\frac{1}{2})^{2m}}{(m!\,)^2} \right)}_{<\infty}.
\end{aligned} \tag{5.6}$$

It follows that

$$\sum_{1\le i\neq k\le N}\ \sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} \left| \sum_{j=1}^{2n+1} \frac{1}{N^2} \frac{G^{\mathrm{I}}_{m,n,j}(x_i)G^{\mathrm{I}}_{m,n,j}(x_k)}{A^2_{m,n}} \right| < +\infty, \tag{5.7}$$

where this convergence is uniform with respect to N, since we find in (5.6) a convergent majorant independent of N. Analogously, computing for the orthonormal basis system of type $\mathrm{X} = \mathrm{II}$ with the help of estimate (1.61) and the summability condition (1.64), we have

$$\begin{aligned}
&\sum_{1\le i\neq k\le N}\ \sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} \left| \sum_{j=1}^{2n+1} \frac{1}{N^2} \frac{G^{\mathrm{II}}_{m,n,j}(x_i)G^{\mathrm{II}}_{m,n,j}(x_k)}{A^2_{m,n}} \right| \\
&\le \frac{N(N-1)}{16\pi R^3 N^2} \left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} \frac{(2n+1)(2m+3)^5}{A^2_{m,n}} \right) \\
&\le \left(1-\frac{1}{N}\right) \left(\frac{1}{16\pi R^3}\right) \left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} \frac{(2n+1)(2m+3)^5}{A^2_{m,n}} \right) \\
&< +\infty.
\end{aligned} \tag{5.8}$$

This completes the proof. ■

Using the previous result, we can now show that the generalized discrepancy actually converges to zero for identically independent random variables. Also the squared discrepancy converges in distribution to the sum of a sequence of random variables.

Theorem 5.1.2 *Let $\mathcal{P}_N = \{x_1, x_2, \ldots, x_N\}$ be a sample of independent and identically distributed uniform random variables on $\mathcal{B}_R$ and $\{A_{m,n}\}$ be the symbol of a pseudodifferential operator $\mathcal{A}$ for any m and n. Further, let the conditions in Theorem 2.2.1 be satisfied. Then the following holds, if $\{A_{m,n}\}$ is summable.*

(i) $D^2(\mathcal{P}_N, \mathcal{A}) \xrightarrow{\text{as}} 0.$

(ii) $N \cdot D^2(\mathcal{P}_N, \mathcal{A}) \xrightarrow{\text{D}} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{3}{4\pi R^3} \frac{\chi^2_{m,n}(2n+1)}{A^2_{m,n}}$,

as $N \to \infty$, where $\chi^2_{m,n}(\mathcal{Z}(d,n))$ are χ^2-random variables with $\mathcal{Z}(d,n)$ degrees of freedom. The convergence 'as' and 'D' are defined by (1.85) *and* (1.86)*, respectively.*

Proof: We know by Definition 2.2.2 of the generalized discrepancy that

$$D^2(\mathcal{P}_N, \mathcal{A}) = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{k=1}^{N} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \sum_{j=1}^{2n+1} \frac{G^{\mathrm{X}}_{m,n,j}(x_i) G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}}.$$

We set

$$h(x_i, x_k) := \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \sum_{j=1}^{2n+1} \frac{G^{\mathrm{X}}_{m,n,j}(x_i) G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}},$$

where $h(x_i, x_k)$ is symmetric. Now, Theorem 1.5.20 tells us that if $\mathbb{E}|h(x_i, x_k)|$ is finite, then the strong law of large numbers holds for $D^2(\mathcal{P}_N, \mathcal{A})$ and

$$D^2(\mathcal{P}_N, \mathcal{A}) = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{k=1}^{N} h(x_i, x_k) \xrightarrow{\text{as}} \int_{\mathcal{B}_R} \int_{\mathcal{B}_R} h(x,y) \mathrm{d}\sigma^*(x) \mathrm{d}\sigma^*(y). \quad (5.9)$$

In order to show that $\mathbb{E}|h(x_i, x_k)| < \infty$, we treat the two cases of types X = I and X = II separately. First, for the type I, we consider the sum

$$\begin{aligned}
&\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \mathbb{E}\left|\sum_{j=1}^{2n+1} \frac{G^{\mathrm{I}}_{m,n,j}(x_i)G^{\mathrm{I}}_{m,n,j}(x_k)}{A^2_{m,n}}\right| \\
&= \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \mathbb{E}\left|\frac{(2n+1)(4m+2l_n+3)}{4\pi R^3 A^2_{m,n}} P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{|x_i|^2}{R^2}-1\right)\right. \\
&\qquad \left. \times P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{|x_k|^2}{R^2}-1\right)\left(\frac{|x_i||x_k|}{R^2}\right)^{l_n} P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\right|.
\end{aligned}$$

With the use of expectation property (1.71), we can write

$$\begin{aligned}
&\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \mathbb{E}\left|\sum_{j=1}^{2n+1} \frac{G^{\mathrm{I}}_{m,n,j}(x_i)G^{\mathrm{I}}_{m,n,j}(x_k)}{A^2_{m,n}}\right| \\
&= \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{(2n+1)(4m+2l_n+3)}{4\pi R^3 A^2_{m,n}} \mathbb{E}\left|P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{|x_i|^2}{R^2}-1\right)\right| \\
&\qquad \times \mathbb{E}\left|P_m^{(0,l_n+\frac{1}{2})}\left(2\frac{|x_k|^2}{R^2}-1\right)\right| \mathbb{E}\left|\left(\frac{|x_i||x_k|}{R^2}\right)^{l_n}\right| \mathbb{E}\left|P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\right|.
\end{aligned}$$

Furthermore, in combination with the monotonicity of expectation (see Theorem 1.5.5), Theorem 1.2.10, the estimate (1.60) and the summability condition (1.63), we deduce

$$\begin{aligned}
&\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \mathbb{E}\left|\sum_{j=1}^{2n+1} \frac{G^{\mathrm{I}}_{m,n,j}(x_i)G^{\mathrm{I}}_{m,n,j}(x_k)}{A^2_{m,n}}\right| \\
&\leq \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{(2n+1)(4m+2l_n+3)}{4\pi R^3 A^2_{m,n}} \frac{\left(m+l_n+\frac{1}{2}\right)^{2m}}{(m!)^2} \\
&< +\infty.
\end{aligned}$$

Similarly, for the system of type X = II with the estimate (1.61) and the summability condition (1.64), we have

$$
\begin{aligned}
&\sum_{(m,n)\neq(0,0)} \mathbb{E}\left|\sum_{j=1}^{2n+1} \frac{G^{\mathrm{II}}_{m,n,j}(x_i)G^{\mathrm{II}}_{m,n,j}(x_k)}{A^2_{m,n}}\right| \\
&= \sum_{(m,n)\neq(0,0)} \mathbb{E}\left|\frac{(2n+1)(2m+3)}{4\pi R^3 A^2_{m,n}} P^{(0,2)}_m\left(2\frac{|x_i|}{R}-1\right) P^{(0,2)}_m\left(2\frac{|x_k|}{R}-1\right)\right. \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \left.\times\, P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\right| \\
&= \sum_{(m,n)\neq(0,0)} \frac{(2n+1)(2m+3)}{4\pi R^3 A^2_{m,n}} \mathbb{E}\left|P^{(0,2)}_m\left(2\frac{|x_i|}{R}-1\right)\right| \mathbb{E}\left|P^{(0,2)}_m\left(2\frac{|x_k|}{R}-1\right)\right| \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \times\, \mathbb{E}\left|P_n\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\right| \\
&\leq \sum_{(m,n)\neq(0,0)} \frac{(2n+1)(2m+3)^5}{16\pi R^3 A^2_{m,n}} \\
&< +\infty.
\end{aligned}
$$

Since the infinite sum of expectations converges in both cases and

$$
\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \sum_{j=1}^{2n+1} \frac{G^{\mathrm{X}}_{m,n,j}(x_i)G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}} < +\infty, \tag{5.10}
$$

from the Minkowski's inequality for expectation (1.78), we can infer

$$
\begin{aligned}
\mathbb{E}|h(x_i,x_k)| &= \mathbb{E}\left|\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \sum_{j=1}^{2n+1} \frac{G^{\mathrm{X}}_{m,n,j}(x_i)G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}}\right| \\
&\leq \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \mathbb{E}\left|\sum_{j=1}^{2n+1} \frac{G^{\mathrm{X}}_{m,n,j}(x_i)G^{\mathrm{X}}_{m,n,j}(x_k)}{A^2_{m,n}}\right|.
\end{aligned} \tag{5.11}
$$

This shows us that the condition for applying Theorem 1.5.20 is fulfilled. We now come back to equation (5.9) and use the orthonormality of the systems

$G^{\mathrm{X}}_{m,n,j}$ to get

$$\begin{aligned}
&\int_{\mathcal{B}_R}\int_{\mathcal{B}_R} h(x,y)\mathrm{d}\sigma^*(x)\mathrm{d}\sigma^*(y) \\
&= \int_{\mathcal{B}_R}\int_{\mathcal{B}_R} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \sum_{j=1}^{2n+1} \frac{G^{\mathrm{X}}_{m,n,j}(x)G^{\mathrm{X}}_{m,n,j}(y)}{A^2_{m,n}}\mathrm{d}\sigma^*(x)\mathrm{d}\sigma^*(y) \qquad (5.12)\\
&= 0,
\end{aligned}$$

which implies that

$$D^2(\mathcal{P}_N,\mathcal{A}) = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{k=1}^{N} h(x_i,x_k) \xrightarrow{\text{as}} 0. \qquad (5.13)$$

This proves the first part. Now for the second part, we consider again the discrepancy

$$D^2(\mathcal{P}_N,\mathcal{A}) = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{k=1}^{N} h(x_i,x_k).$$

Since $h(x_i,x_k)$ is symmetric, we can rewrite it as

$$D^2(\mathcal{P}_N,\mathcal{A}) = \frac{1}{N^2}\sum_{i\neq k} h(x_i,x_k) + \frac{1}{N^2}\sum_{i=1}^{N} h(x_i,x_i). \qquad (5.14)$$

We will now consider the first sum on the right hand side in (5.14), which is a U-statistics by Definition 1.5.17, i.e.

$$NU_N = \frac{1}{N}\sum_{i\neq k} h(x_i,x_k).$$

For all $i<k$, the symmetric property of h allows us to rewrite the above equation as

$$\frac{N}{N-1}U_N = \frac{2}{N(N-1)}\sum_{i<k} h(x_i,x_k),$$

Since $\mathbb{E}[h(x,y)] = \int_{\mathcal{B}_R} h(x,y)\mathrm{d}\sigma^*(y) = 0$ (where x is kept fixed and the expectation is taken with respect to random variable y), according to Definition 1.5.19 we can say that h is a 1-degenerate kernel and U_N is a degenerate U-statistics. Now, using the idea of asymptotic distribution of degenerate

U-statistics from [41, 62], we can find the limit distribution of U_N. We approximate U_N

$$\frac{N}{N-1}U_N = \frac{2}{N(N-1)}\sum_{i<k}\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} A_{m,n}^{-2}\sum_{j=1}^{2n+1} G_{m,n,j}^{\mathrm{X}}(x_i)G_{m,n,j}^{\mathrm{X}}(x_k)$$

by U_N^M, such that

$$\frac{N}{N-1}U_N^M = \frac{2}{N(N-1)}\sum_{i<k}\sum_{\substack{(m,n)\neq(0,0)\\ m+n\leq M,\, l_n\geq 0}} A_{m,n}^{-2}\sum_{j=1}^{2n+1} G_{m,n,j}^{\mathrm{X}}(x_i)G_{m,n,j}^{\mathrm{X}}(x_k).$$

Rewriting the equation above, we have

$$NU_N^M = \sum_{\substack{(m,n)\neq(0,0)\\ m+n\leq M,\, l_n\geq 0}}\sum_{j=1}^{2n+1} A_{m,n}^{-2}\left[\left(\frac{1}{\sqrt{N}}\sum_{i=1}^{N} G_{m,n,j}^{\mathrm{X}}(x_i)\right)^2 - \frac{1}{N}\sum_{i=1}^{N}\left(G_{m,n,j}^{\mathrm{X}}(x_i)\right)^2\right]. \tag{5.15}$$

Since the x_i's are independent and identically distributed on $\mathcal{B}_R$ and in accordance with equations (5.1) and (5.2) the conditions on function $G_{m,n,j}^{\mathrm{X}}$ are satisfied, we can use the central limit theorem 1.5.21 for the first term in (5.15)

$$\frac{1}{\sqrt{N}}\sum_{i=1}^{N} G_{m,n,j}^{\mathrm{X}}(x_i) \xrightarrow{\mathrm{D}} \sqrt{\frac{3}{4\pi R^3}}Z,$$

where Z is a standard normal random variable and $\frac{3}{4\pi R^3}$ is the variance of function $G_{m,n,j}^{\mathrm{X}}$ (see equation (5.1)). Further, by the strong law of large numbers 1.5.20, the second term in (5.15) converges '*almost surely*' to the variance of $G_{m,n,j}^{\mathrm{X}}(x)$, i.e.

$$\frac{1}{N}\sum_{i=1}^{N}\left(G_{m,n,j}^{\mathrm{X}}(x_i)\right)^2 \xrightarrow{\mathrm{as}} \frac{3}{4\pi R^3}. \tag{5.16}$$

From Remark 1.5.15, we already know that almost sure convergence implies convergence in probability for (5.16). Hence, Slutsky's theorem 1.5.16 shows that U_N^M also converges '*in distribution*' as follows

$$NU_N^M \xrightarrow{\mathrm{D}} \frac{3}{4\pi R^3}\sum_{\substack{(m,n)\neq(0,0)\\ m+n\leq M,\, l_n\geq 0}}\sum_{j=1}^{2n+1} A_{m,n}^{-2}\left(Z_{m,n,j}^2 - 1\right).$$

As $M \to \infty$, we finally get

$$NU_N \xrightarrow{\mathrm{D}} \frac{3}{4\pi R^3} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \sum_{j=1}^{2n+1} A_{m,n}^{-2}\left(Z_{m,n,j}^2 - 1\right)$$

(see [41, 62]). Here, the presence of the term $\frac{3}{4\pi R^3}$ is due to the orthonormality of the systems $\{G_{m,n,j}^{\mathrm{X}}\}$ with respect to the measure σ^*. Now, from Definition 1.5.8, a single squared standard normal variable can be written as a χ^2-random variable of degree of freedom one (Note that, the degree of freedom denotes here the number of 'independent' normal random variables) i.e. $Z^2 = \chi^2(1)$, so we have $\sum_{j=1}^{2n+1} Z_{m,n,j}^2 = \chi_{m,n}^2(2n+1)$, where $\chi_{m,n}^2(\mathcal{Z}(d,n))$ is a χ^2-random variable with indices m, n and degrees of freedom $\mathcal{Z}(d,n)$. This gives us

$$NU_N \xrightarrow{\mathrm{D}} \frac{3}{4\pi R^3} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} A_{m,n}^{-2}\left(\chi_{m,n}^2(2n+1) - (2n+1)\right). \tag{5.17}$$

Now, we come to the second term in (5.15), which converges *'almost surely'* to $\mathbb{E}\left[h(x,x)\right]$ by the strong law of large numbers 1.5.20. The expectation of $h(x,x)$ can be calculated as

$$\begin{aligned}\mathbb{E}\left[h(x,x)\right] &= \int_{\mathcal{B}_R} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \sum_{j=1}^{2n+1} \frac{1}{A_{m,n}^2}\left(G_{m,n,j}^{\mathrm{X}}(x)\right)^2 \mathrm{d}\sigma^*(x)\\ &= \frac{3}{4\pi R^3} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{2n+1}{A_{m,n}^2}. \end{aligned} \tag{5.18}$$

By combining equations (5.17) and (5.18), we immediately get

$$N \cdot D^2(\mathcal{P}_N, \mathcal{A}) \xrightarrow{\mathrm{D}} \frac{3}{4\pi R^3} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} A_{m,n}^{-2}\left(\chi_{m,n}^2(2n+1)\right),$$

as required. ■

From the previous theorem, it is also easy to deduce the expectation of the generalized discrepancy. By using equations (5.12), (5.18) and the linearity of expectation (1.74) in (5.14) for x_i's $\in \mathcal{P}_N$, we obtain

$$\mathbb{E}\left[D^2(\mathcal{P}_N, \mathcal{A})\right] = \frac{3}{4\pi N R^3} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{2n+1}{A_{m,n}^2}. \tag{5.19}$$

5.2 Computation of Asymptotic Distribution

In the succeeding results, we denote the asymptotic distribution of $N \cdot D^2(\omega_N, \mathcal{A})$, calculated in the previous section, by

$$\mathcal{Y} = \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{3}{4\pi R^3} \frac{\chi^2_{m,n}(2n+1)}{A^2_{m,n}}. \tag{5.20}$$

In this section, we consider two methods, in analogy to the spherical case [11], for approximating this asymptotic distribution. The first approximation of $\mathcal{Y}$ is the truncated version $\mathcal{Y}_\nu$, which is obtained simply by taking finite sums in $\mathcal{Y}$, i.e.

$$\mathcal{Y}_\nu = \sum_{\substack{m+n\leq\nu,\, l_n\geq 0\\ (m,n)\neq(0,0)}} \frac{3}{4\pi R^3} \frac{\chi^2_{m,n}(2n+1)}{A^2_{m,n}}. \tag{5.21}$$

The other approximation, named as the centred version, of the distribution $\mathcal{Y}$ is obtained by shifting the truncated version $\mathcal{Y}_\nu$ by adding a constant term C_ν, i.e.

$$\begin{aligned}\mathcal{Y}^*_\nu &= \sum_{\substack{m+n\leq\nu,\, l_n\geq 0\\ (m,n)\neq(0,0)}} \frac{3}{4\pi R^3} \frac{\chi^2_{m,n}(2n+1)}{A^2_{m,n}} + C_\nu,\\ &= \mathcal{Y}_\nu + C_\nu, \end{aligned} \tag{5.22}$$

where

$$C_\nu = \sum_{\substack{m+n>\nu\\ l_n\geq 0}} \frac{3}{4\pi R^3} \frac{2n+1}{A^2_{m,n}}. \tag{5.23}$$

In particular, for the case where $A_{m,n} = (\mathbb{A}^{p,q}_{\mathrm{X}})^\wedge(m,n)$ (defined in (2.9) and (2.10) for X = I and X = II, respectively) with $p = \frac{1}{2}$, $q = \frac{3}{4}$ and for X = I, we have the following representation of C_ν:

$$\frac{3}{4\pi R^3} \sum_{\substack{m+n>\nu\\ l_n\geq 0}} \frac{2n+1}{\left((\mathbb{A}^{p,q}_{\mathrm{I}})^\wedge(m,n)\right)^2} = \frac{3}{4\pi R^3} \sum_{\substack{m+n>\nu\\ l_n\geq 0}} \frac{8}{(4m+2l_n+3)^3\, n(n+1)} \tag{5.24}$$

and for X = II, we have

$$\frac{3}{4\pi R^3} \sum_{m+n>\nu} \frac{2n+1}{\left((\mathbb{A}^{p,q}_{\mathrm{II}})^\wedge(m,n)\right)^2} = \frac{3}{4\pi R^3} \sum_{m+n>\nu} \frac{8}{(2m+3)^3 n(n+1)}.$$

Now, we state the following result related to the approximations of $\mathcal{Y}$ for the later use.

Theorem 5.2.1 *Let $\mathcal{Y}$, $\mathcal{Y}_\nu$ and $\mathcal{Y}_\nu^*$ be as defined by* (5.20), (5.21) *and* (5.22), *respectively, then the following holds true:*

1. $\mathbb{E}(\mathcal{Y}) = \mathbb{E}(\mathcal{Y}_\nu^*)$.
2. $\mathbb{V}(\mathcal{Y} - \mathcal{Y}_\nu^*) = \mathbb{V}(\mathcal{Y} - \mathcal{Y}_\nu)$.
3. $|\phi_{\mathcal{Y}_\nu}(t)| = \left|\phi_{\mathcal{Y}_\nu^*}(t)\right|$.

Proof:

1. In accordance with (5.20), (1.75) and Theorem 1.5.11, the expectation of $\mathcal{Y}$ is computed as

$$\begin{aligned}
\mathbb{E}(\mathcal{Y}) &= \mathbb{E}\left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{3}{4\pi R^3}\frac{\chi^2_{m,n}(2n+1)}{A^2_{m,n}}\right)\\
&= \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{3}{4\pi R^3}\frac{1}{A^2_{m,n}}\mathbb{E}\left(\chi^2_{m,n}(2n+1)\right)\\
&= \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{3}{4\pi R^3}\frac{2n+1}{A^2_{m,n}}.
\end{aligned}$$

Next, calculating the expectation of $\mathcal{Y}_\nu^*$, we get

$$\mathbb{E}(\mathcal{Y}_\nu^*) = \mathbb{E}\left(\sum_{\substack{m+n\leq\nu,\, l_n\geq 0\\ (m,n)\neq(0,0)}} \frac{3}{4\pi R^3}\frac{\chi^2_{m,n}(2n+1)}{A^2_{m,n}} + \sum_{\substack{m+n>\nu\\ l_n\geq 0}} \frac{3}{4\pi R^3}\frac{2n+1}{A^2_{m,n}}\right).$$

Let us now use the linearity of expectation (1.75) for the above sum. Then the above equation yields

$$\begin{aligned}
\mathbb{E}(\mathcal{Y}_\nu^*) &= \sum_{\substack{m+n\leq\nu,\, l_n\geq 0\\ (m,n)\neq(0,0)}} \frac{3}{4\pi R^3}\frac{2n+1}{A^2_{m,n}} + \sum_{\substack{m+n>\nu\\ l_n\geq 0}} \frac{3}{4\pi R^3}\frac{2n+1}{A^2_{m,n}}\\
&= \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{3}{4\pi R^3}\frac{2n+1}{A^2_{m,n}}.
\end{aligned}$$

This gives us the required result.

2. From (5.22), we already know that $\mathcal{Y} - \mathcal{Y}_\nu^* = \mathcal{Y} - \mathcal{Y}_\nu - C_\nu$. Hence, the variance of term $\mathcal{Y} - \mathcal{Y}_\nu^*$ is given by

$$\mathbb{V}\left(\mathcal{Y} - \mathcal{Y}_\nu^*\right) = \mathbb{V}\left(\mathcal{Y} - \mathcal{Y}_\nu - C_\nu\right).$$

Since C_ν is a constant term, using (1.73), we get

$$\mathbb{V}\left(\mathcal{Y} - \mathcal{Y}_\nu^*\right) = \mathbb{V}\left(\mathcal{Y} - \mathcal{Y}_\nu\right). \tag{5.25}$$

3. According to the Definition 1.5.9, the characteristic function of $\mathcal{Y}_\nu^*$ is given as

$$\phi_{\mathcal{Y}_\nu^*}(t) = \mathbb{E}\left(e^{it\mathcal{Y}_\nu^*}\right).$$

With the use of equation (5.22), we obtain

$$\begin{aligned}\phi_{\mathcal{Y}_\nu^*}(t) &= \mathbb{E}\left(e^{it(\mathcal{Y}_\nu + C_\nu)}\right)\\ &= e^{itC_\nu}\mathbb{E}\left(e^{it\mathcal{Y}_\nu}\right),\end{aligned}$$

where $C_\nu = \sum_{\substack{m+n>\nu\\ l_n \geq 0}} \frac{3}{4\pi R^3}\frac{2n+1}{A_{m,n}^2}$ and since $|e^{itC_\nu}| = 1$, we obtain

$$\begin{aligned}\left|\phi_{\mathcal{Y}_\nu^*}(t)\right| &= \left|e^{itC_\nu}\right| \left|\phi_{\mathcal{Y}_\nu}(t)\right|\\ &= \left|\phi_{\mathcal{Y}_\nu}(t)\right|,\end{aligned}$$

as required.

■

The following result calculates the error bound between $\mathcal{Y}$ and its approximations.

Theorem 5.2.2 *For $m, n \in \mathbb{N}_0$ with $(m, n) \neq (0, 0)$ and $l_n \geq 0$, the following holds:*

$$\begin{aligned}&\left|\mathbb{P}\{\mathcal{Y} \leq y\} - \mathbb{P}\{\mathcal{Y}_\nu \leq y\}\right|\\ &\quad\leq \sqrt{\frac{2\sum_{m+n>\nu}\frac{2n+1}{A_{m,n}^4} + \left(\sum_{m+n>\nu}\frac{2n+1}{A_{m,n}^2}\right)^2}{\sum_{\substack{m+n\leq\nu\\ n\neq 0}}\frac{2n+1}{A_{m,n}^4}}} \cdot \frac{\sqrt{3}}{2\pi} \cdot \mathrm{B}\left(\frac{1}{2}, \frac{1}{4}\right),\end{aligned} \tag{5.26}$$

where B *is the Beta function and*

$$\left|\mathbb{P}\{\mathcal{Y} \leq y\} - \mathbb{P}\{\mathcal{Y}_\nu^* \leq y\}\right| \leq \frac{\sum_{m+n>\nu}\frac{2n+1}{A_{m,n}^4}}{\sum_{\substack{m+n\leq\nu\\ n\notin\{0,1\}}}\frac{2n+1}{A_{m,n}^4}} \cdot \frac{5}{\pi}. \tag{5.27}$$

Proof: By the inversion formula (see Theorem 1.5.12), we have

$$|\mathbb{P}\{\mathcal{Y} \leq y\} - \mathbb{P}\{\mathcal{Y}_\nu \leq y\}| = \frac{1}{2\pi} \left| \int_0^x \int_{-\infty}^{\infty} [\phi_{\mathcal{Y}}(t) - \phi_{\mathcal{Y}_\nu}(t)]\, e^{-its}\, \mathrm{d}t\, \mathrm{d}s \right| \tag{5.28}$$

Since

$$\int_0^x e^{-its}\, \mathrm{d}s = \frac{1}{it}(1 - e^{-itx}),$$

then with $|1 - e^{-itx}| \leq 2$, equation (5.28) yields

$$\begin{aligned} |\mathbb{P}\{\mathcal{Y} \leq y\} - \mathbb{P}\{\mathcal{Y}_\nu \leq y\}| &\leq \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{|t|} |\phi_{\mathcal{Y}}(t) - \phi_{\mathcal{Y}_\nu}(t)| \left|1 - e^{-itx}\right| \mathrm{d}t \\ &\leq \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{|t|} |\phi_{\mathcal{Y}}(t) - \phi_{\mathcal{Y}_\nu}(t)|\, \mathrm{d}t \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{|t|} |\phi_{\mathcal{Y}_\nu}(t)| \left| \frac{\phi_{\mathcal{Y}_\nu + \mathcal{Y} - \mathcal{Y}_\nu}(t)}{\phi_{\mathcal{Y}_\nu}(t)} - 1 \right| \mathrm{d}t \end{aligned} \tag{5.29}$$

Since $\mathcal{Y}_\nu$ and $\mathcal{Y} - \mathcal{Y}_\nu$ are independent, so due to Theorem 1.5.10, the characteristic function of the random variable $\mathcal{Y}_\nu + \mathcal{Y} - \mathcal{Y}_\nu$ is the product of characteristic functions of $\mathcal{Y}_\nu$ and $\mathcal{Y} - \mathcal{Y}_\nu$. So we can write as follows

$$\frac{\phi_{\mathcal{Y}_\nu + \mathcal{Y} - \mathcal{Y}_\nu}(t)}{\phi_{\mathcal{Y}_\nu}(t)} = \frac{\phi_{\mathcal{Y}_\nu}(t) \cdot \phi_{\mathcal{Y} - \mathcal{Y}_\nu}(t)}{\phi_{\mathcal{Y}_\nu}(t)} = \phi_{\mathcal{Y} - \mathcal{Y}_\nu}(t) = \mathbb{E}\left(e^{it(\mathcal{Y} - \mathcal{Y}_\nu)}\right)$$

This reduces (5.29) to the following inequality:

$$\begin{aligned} |\mathbb{P}\{\mathcal{Y} \leq y\} - \mathbb{P}\{\mathcal{Y}_\nu \leq y\}| &\leq \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{|t|} |\phi_{\mathcal{Y}_\nu}(t)| \left| \mathbb{E}\left(e^{it(\mathcal{Y} - \mathcal{Y}_\nu)}\right) - 1 \right| \mathrm{d}t \\ &\leq \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{|t|} |\phi_{\mathcal{Y}_\nu}(t)|\, \mathbb{E}|e^{it(\mathcal{Y} - \mathcal{Y}_\nu)} - 1| \mathrm{d}t. \end{aligned}$$

Since

$$\left| e^{it(\mathcal{Y} - \mathcal{Y}_\nu)} - 1 \right| = \left| \int_0^{t(\mathcal{Y} - \mathcal{Y}_\nu)} i e^{is} \mathrm{d}s \right| \leq \int_0^{t(\mathcal{Y} - \mathcal{Y}_\nu)} \mathrm{d}s = |t||\mathcal{Y} - \mathcal{Y}_\nu|$$

(see [62, 63]) and from Cauchy-Schwarz inequality (1.77)

$$\mathbb{E}\,|\mathcal{Y} - \mathcal{Y}_\nu| \leq \sqrt{\mathbb{E}(\mathcal{Y} - \mathcal{Y}_\nu)^2},$$

hence, we have

$$|\mathbb{P}\{\mathcal{Y} \leq y\} - \mathbb{P}\{\mathcal{Y}_\nu \leq y\}| \leq \frac{1}{\pi} \sqrt{\mathbb{E}(\mathcal{Y} - \mathcal{Y}_\nu)^2} \int_{-\infty}^{\infty} |\phi_{\mathcal{Y}_\nu}(t)|\, \mathrm{d}t. \tag{5.30}$$

The above inequality requires further the computation of two terms, that are: the expectation of the random variable $(\mathcal{Y}-\mathcal{Y}_\nu)^2$ and the characteristic function of the variable $\mathcal{Y}_\nu$. Firstly, we compute the expectation of $(\mathcal{Y}-\mathcal{Y}_\nu)^2$.

$$\begin{aligned}\mathbb{E}(\mathcal{Y}-\mathcal{Y}_\nu)^2 &= \mathbb{E}\left(\sum_{m+n>\nu}\frac{3}{4\pi R^3}\frac{\chi^2_{m,n}(2n+1)}{A^2_{m,n}}\right)^2\\ &= \left(\mathbb{E}\left(\sum_{m+n>\nu}\frac{3}{4\pi R^3}\frac{\chi^2_{m,n}(2n+1)}{A^2_{m,n}}\right)\right)^2\\ &\quad+\mathbb{V}\left(\sum_{m+n>\nu}\frac{3}{4\pi R^3}\frac{\chi^2_{m,n}(2n+1)}{A^2_{m,n}}\right). \end{aligned} \tag{5.31}$$

We use first the linearity of expectation (1.75) and the property (1.73) of the variance to get

$$\begin{aligned}\mathbb{E}(\mathcal{Y}-\mathcal{Y}_\nu)^2 = &\left(\sum_{m+n>\nu}\frac{3}{4\pi R^3}\frac{1}{A^2_{m,n}}\mathbb{E}(\chi^2_{m,n}(2n+1))\right)^2\\ &+\sum_{m+n>\nu}\frac{9}{16\pi^2R^6}\frac{1}{A^4_{m,n}}\mathbb{V}(\chi^2_{m,n}(2n+1)).\end{aligned}$$

Furthermore, Theorem 1.5.11 for χ^2- random variables implies that

$$\mathbb{E}(\mathcal{Y}-\mathcal{Y}_\nu)^2 = \left(\sum_{m+n>\nu}\frac{3}{4\pi R^3}\frac{2n+1}{A^2_{m,n}}\right)^2+\sum_{m+n>\nu}\frac{9}{16\pi^2R^6}\frac{2(2n+1)}{A^4_{m,n}}. \tag{5.32}$$

Next, we calculate the characteristic function of $\mathcal{Y}_\nu = \sum_{m+n\le\nu}\frac{3}{4\pi R^3}\frac{\chi^2_{m,n}(2n+1)}{A^2_{m,n}}$. By virtue of Theorem 1.5.10, the characteristic function of $\mathcal{Y}_\nu$ is as follows

$$\phi_{\mathcal{Y}_\nu}(t) = \prod_{\substack{m+n\le\nu\\(m,n)\neq(0,0)}}\phi_{\chi^2_{m,n}(2n+1)}\left(\frac{3}{4\pi R^3A^2_{m,n}}t\right).$$

We apply equation (1.82) for the characteristic functions of χ^2-random variables with n degrees of freedom and obtain

$$\begin{aligned}\phi_{\mathcal{Y}_\nu}(t) &= \prod_{\substack{m+n\leq\nu\\(m,n)\neq(0,0)}} \left(1-\frac{3}{2\pi R^3 A_{m,n}^2}it\right)^{-\frac{2n+1}{2}}\\ &= \exp\left(-\sum_{\substack{m+n\leq\nu\\(m,n)\neq(0,0)}} \frac{2n+1}{2}\ln\left(1-\frac{3}{2\pi R^3 A_{m,n}^2}it\right)\right).\end{aligned}$$

Further, we use the identity $\ln(x+iy) = \ln\sqrt{x^2+y^2} + i\arctan\left(\frac{y}{x}\right)$, $x, y \in \mathbb{R}$ such that $-\pi < \arctan\left(\frac{y}{x}\right) \leq \pi$, from [1] and get

$$\begin{aligned}\phi_{\mathcal{Y}_\nu}(t) = \exp\Bigg(&-\sum_{\substack{m+n\leq\nu\\(m,n)\neq(0,0)}} \frac{2n+1}{2}\ln\sqrt{1+\frac{9}{4\pi^2R^6A_{m,n}^4}t^2}\\ &-i\sum_{\substack{m+n\leq\nu\\(m,n)\neq(0,0)}} \frac{2n+1}{2}\arctan\left(\frac{-3t}{2\pi R^3 A_{m,n}^2}\right)\Bigg).\end{aligned}$$

The imaginary part in the above equation vanishes after taking the absolute value of the characteristic function, which yields

$$\begin{aligned}|\phi_{\mathcal{Y}_\nu}(t)| &= \exp\left(-\sum_{\substack{m+n\leq\nu\\(m,n)\neq(0,0)}} \frac{2n+1}{2}\ln\sqrt{1+\frac{9}{4\pi^2R^6A_{m,n}^4}t^2}\right)\\ &= \prod_{\substack{m+n\leq\nu\\(m,n)\neq(0,0)}} \left(1+\frac{9}{4\pi^2R^6A_{m,n}^4}t^2\right)^{-\frac{2n+1}{4}}.\end{aligned}$$

Additionally, we exclude all the factors with $n = 0$ in order to get the following form:

$$
\begin{aligned}
|\phi_{\mathcal{Y}_\nu}(t)| &\le \frac{1}{\prod\limits_{\substack{m+n\le\nu\\ n\neq 0}} \left(1 + \frac{9}{4\pi^2 R^6 A_{m,n}^4} t^2\right)^{\frac{2n+1}{4}}} \\
&= \frac{1}{\prod\limits_{\substack{m+n\le\nu\\ n\neq 0}} \left(\left(1 + \frac{9}{4\pi^2 R^6 A_{m,n}^4} t^2\right)^{\frac{2n+1}{3}}\right)^{\frac{3}{4}}}.
\end{aligned} \tag{5.33}
$$

Using Bernoulli's inequality, we get the following inequality for the characteristic function of $\mathcal{Y}_\nu$.

$$
|\phi_{\mathcal{Y}_\nu}(t)| \le \frac{1}{\left(1 + \sum\limits_{\substack{m+n\le\nu\\ n\neq 0}} \frac{3}{4\pi^2 R^6} \frac{2n+1}{A_{m,n}^4} t^2\right)^{\frac{3}{4}}}. \tag{5.34}
$$

In accordance with equation (5.32) and inequality (5.34), (5.30) becomes

$$
|\mathbb{P}\{\mathcal{Y} \le y\} - \mathbb{P}\{\mathcal{Y}_\nu \le y\}| \le \frac{\sqrt{\left(\sum\limits_{m+n>\nu} \frac{3}{4\pi R^3} \frac{2n+1}{A_{m,n}^2}\right)^2 + \left(\sum\limits_{m+n>\nu} \frac{9}{16\pi^2 R^6} \frac{2(2n+1)}{A_{m,n}^4}\right)}}{\pi} \times \int_{-\infty}^{\infty} \frac{\mathrm{d}t}{\left(1 + \sum\limits_{\substack{m+n\le\nu\\ n\neq 0}} \frac{3}{4\pi^2 R^6} \frac{2n+1}{A_{m,n}^4} t^2\right)^{\frac{3}{4}}}.
$$

For simplifying the integral in the above inequality, we substitute

$$
z = \sum_{\substack{m+n\le\nu\\ n\neq 0}} \frac{3}{4\pi^2 R^6} \frac{2n+1}{A_{m,n}^4} t^2
$$

with

$$
\mathrm{d}t = \frac{\mathrm{d}z}{2\sqrt{z}} \frac{1}{\sqrt{\sum\limits_{\substack{m+n\le\nu\\ n\neq 0}} \frac{3}{4\pi^2 R^6} \frac{2n+1}{A_{m,n}^4}}},
$$

and get the following inequality:

$$
\begin{aligned}
&|\mathbb{P}\{\mathcal{Y} \leq y\} - \mathbb{P}\{\mathcal{Y}_\nu \leq y\}| \\
&\leq \frac{1}{\pi}\sqrt{\frac{\left(\sum\limits_{m+n>\nu} \frac{3}{4\pi R^3}\frac{2n+1}{A_{m,n}^2}\right)^2 + \left(\sum\limits_{m+n>\nu} \frac{9}{16\pi^2 R^6}\frac{2(2n+1)}{A_{m,n}^4}\right)}{\sum\limits_{\substack{m+n\leq\nu\\ n\neq 0}} \frac{3}{4\pi^2 R^6}\frac{2n+1}{A_{m,n}^4}}}\int\limits_0^\infty \frac{\mathrm{d}z}{z^{\frac{1}{2}}(1+z)^{\frac{3}{4}}} \\
&\leq \sqrt{\frac{\left(\sum\limits_{m+n>\nu}\frac{2n+1}{A_{m,n}^2}\right)^2 + 2\sum\limits_{m+n>\nu}\frac{2n+1}{A_{m,n}^4}}{\sum\limits_{\substack{m+n\leq\nu\\ n\neq 0}}\frac{2n+1}{A_{m,n}^4}}}\cdot\frac{\sqrt{3}}{2\pi}\cdot \mathrm{B}\left(\frac{1}{2},\frac{1}{4}\right),
\end{aligned}
$$

where the beta function B is given by Definition 1.1.5. Next, we have to derive the error bound for the centred version $\mathcal{Y}_\nu^*$. From Theorem 5.2.1, it is clear that $|\phi_{\mathcal{Y}_\nu^*}|=|\phi_{\mathcal{Y}_\nu}|$. So, the inequality (5.33) implies that

$$
\begin{aligned}
\left|\phi_{\mathcal{Y}_\nu^*}(t)\right| &\leq \frac{1}{\prod\limits_{\substack{m+n\leq\nu\\ n\neq 0}}\left(1+\frac{9}{4\pi^2R^6A_{m,n}^4}t^2\right)^{\frac{2n+1}{4}}} \\
&= \frac{1}{\prod\limits_{m=0}^{\nu-1}\left(1+\frac{9}{4\pi^2R^6A_{m,1}^4}t^2\right)^{\frac{3}{4}}\cdot\prod\limits_{\substack{m+n\leq\nu\\ n\notin\{0,1\}}}\left(1+\frac{9}{4\pi^2R^6A_{m,n}^4}t^2\right)^{\frac{2n+1}{4}}}.
\end{aligned}
$$

Ignoring the factors with $n=1$, we obtain

$$
\begin{aligned}
\left|\phi_{\mathcal{Y}_\nu^*}(t)\right| &\leq \frac{1}{\prod\limits_{\substack{m+n\leq\nu\\ n\notin\{0,1\}}}\left(1+\frac{9}{4\pi^2R^6A_{m,n}^4}t^2\right)^{\frac{2n+1}{4}}} \\
&= \frac{1}{\prod\limits_{\substack{m+n\leq\nu\\ n\notin\{0,1\}}}\left(\left(1+\frac{9}{4\pi^2R^6A_{m,n}^4}t^2\right)^{\frac{2n+1}{5}}\right)^{\frac{5}{4}}}.
\end{aligned}
$$

Finally, with the use of Bernoulli's inequality as above, we get

$$
\left|\phi_{\mathcal{Y}_\nu^*}(t)\right| \leq \frac{1}{\left(1+t^2\sum\limits_{\substack{m+n\leq\nu\\ n\notin\{0,1\}}}\frac{9}{20\pi^2R^6}\frac{2n+1}{A_{m,n}^4}\right)^{\frac{5}{4}}}. \tag{5.35}
$$

Now using Lemma 1.5.13 and the fact that $\mathbb{E}(\mathcal{Y}) = \mathbb{E}(\mathcal{Y}_\nu^*)$, $|\mathbb{E}e^{it(\mathcal{Y}-\mathcal{Y}_\nu^*)} - 1|$ becomes

$$\begin{aligned}\left|\mathbb{E}e^{it(\mathcal{Y}-\mathcal{Y}_\nu^*)} - 1\right| &= \left|\mathbb{E}e^{it(\mathcal{Y}-\mathcal{Y}_\nu^*)} - 1 - \mathbb{E}it(\mathcal{Y}-\mathcal{Y}_\nu^*)\right| \\ &\le \mathbb{E}\left|e^{it(\mathcal{Y}-\mathcal{Y}_\nu^*)} - 1 - it(\mathcal{Y}-\mathcal{Y}_\nu^*)\right| \\ &\le \frac{1}{2}|t|^2\,\mathbb{E}\left(\mathcal{Y}-\mathcal{Y}_\nu^*\right)^2 \\ &= \frac{1}{2}|t|^2\,\mathbb{V}\left(\mathcal{Y}-\mathcal{Y}_\nu^*\right).\end{aligned}$$

From (5.25), we know that $\mathbb{V}(\mathcal{Y}-\mathcal{Y}_\nu^*) = \mathbb{V}(\mathcal{Y}-\mathcal{Y}_\nu)$, where the variance of $\mathcal{Y}-\mathcal{Y}_\nu$ has already been calculated in (5.32). This implies

$$\left|\mathbb{E}e^{it(\mathcal{Y}-\mathcal{Y}_\nu^*)} - 1\right| = \frac{1}{2}|t|^2 \sum_{m+n>\nu} \frac{9}{16\pi^2 R^6}\frac{2(2n+1)}{A_{m,n}^4}. \tag{5.36}$$

Combining the calculations from equations (5.35) and (5.36), we arrive at

$$\begin{aligned}&|\mathbb{P}\{\mathcal{Y}\le y\} - \mathbb{P}\{\mathcal{Y}_\nu^*\le y\}| \\ &\le \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{1}{|t|}\left|\phi_{\mathcal{Y}_\nu^*}(t)\right|\left|\mathbb{E}e^{it(\mathcal{Y}-\mathcal{Y}_\nu^*)} - 1\right|\mathrm{d}t \\ &\le \frac{2}{\pi}\sum_{m+n>\nu}\frac{9}{16\pi^2R^6}\frac{2n+1}{A_{m,n}^4}\int_0^\infty \frac{t\,\mathrm{d}t}{\left(1+t^2\sum\limits_{\substack{m+n\le\nu\\ n\notin\{0,1\}}}\frac{9}{20\pi^2R^6}\frac{2n+1}{A_{m,n}^4}\right)^{\frac{5}{4}}}.\end{aligned}$$

We substitute $z = t^2 \sum\limits_{\substack{m+n\le\nu\\ n\notin\{0,1\}}} \frac{9}{20\pi^2R^6}\frac{2n+1}{A_{m,n}^4}$, with $t\,\mathrm{d}t = \frac{\mathrm{d}z}{2}\frac{1}{\sum\limits_{\substack{m+n\le\nu\\ n\notin\{0,1\}}} \frac{9}{20\pi^2R^6}\frac{2n+1}{A_{m,n}^4}}$ and consequently get

$$\begin{aligned}|\mathbb{P}\{\mathcal{Y}\le y\} - \mathbb{P}\{\mathcal{Y}_\nu^*\le y\}| &\le \frac{\sum\limits_{m+n>\nu}\frac{9}{16\pi^2R^6}\frac{2n+1}{A_{m,n}^4}}{\sum\limits_{\substack{m+n\le\nu\\ n\notin\{0,1\}}}\frac{9}{20\pi^2R^6}\frac{2n+1}{A_{m,n}^4}}\frac{1}{\pi}\int_0^\infty\frac{\mathrm{d}z}{(1+z)^{\frac{5}{4}}} \\ &\le \frac{\sum\limits_{m+n>\nu}\frac{2n+1}{A_{m,n}^4}}{\sum\limits_{\substack{m+n\le\nu\\ n\notin\{0,1\}}}\frac{2n+1}{A_{m,n}^4}}\cdot\frac{5}{4\pi}\cdot \mathrm{B}\left(1,\frac{1}{4}\right).\end{aligned}$$

Observing that

$$\mathrm{B}\left(1,\frac{1}{4}\right) = \frac{\Gamma(1)\Gamma(1/4)}{\Gamma(5/4)} = \frac{\Gamma(1/4)}{(1/4)\Gamma(1/4)} = 4$$

(see Theorem 1.1.6), we get the desired result. ■
e

Chapter 6

Generalization to Higher Dimensions

The equidistribution theory on the 3-dimensional ball can be generalized to higher dimensions $d \geq 3$, i.e. to the d-dimensional ball $\mathcal{B}_R^d \subset \mathbb{R}^d$. For this purpose, we need to construct orthonormal systems and Sobolev spaces for d dimensions. Some of the papers that discuss Sobolev spaces and their characterizations in arbitrary dimensions on the sphere are [6, 8, 40]. A generalization of classical orthogonal polynomials and a construction of orthonormal bases for Sobolev spaces in higher dimensions can be found, for example, in [17], however, in this chapter, we construct new orthonormal basis systems for $\mathrm{L}^2(\mathcal{B}_R^d)$. This chapter also includes the generalization of spherical harmonics and the related results ([19, 53]), a derivation of differential operators for the constructed orthonormal systems and a formulation of Sobolev spaces defined on $\mathcal{B}_R^d$. We start the chapter with some basics.

6.1 Basic Notations

Definition 6.1.1 *For radius R and dimension $d \geq 3$, the volume of the ball $\mathcal{B}_R^d$ is given by*

$$\sigma_d := \int_0^R r^{d-1} \int_{\Omega^{d-1}} \mathrm{d}\omega(\xi)\,\mathrm{d}r = \frac{\pi^{\frac{d}{2}} R^d}{\Gamma\left(1+\frac{d}{2}\right)} \tag{6.1}$$

and the surface area of Ω^{d-1} is

$$\omega_d := \left.\frac{\mathrm{d}\sigma_d}{\mathrm{d}R}\right|_{R=1} = \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)}. \tag{6.2}$$

Theorem 6.1.2 *Let*

$$\begin{aligned} x_1 &= r \sin\theta_{d-2} \sin\theta_{d-3} \ldots \sin\theta_2 \sin\theta_1 \sin\phi, \\ x_2 &= r \sin\theta_{d-2} \sin\theta_{d-3} \ldots \sin\theta_2 \sin\theta_1 \cos\phi, \\ x_3 &= r \sin\theta_{d-2} \sin\theta_{d-3} \ldots \sin\theta_2 \cos\theta_1, \\ &\vdots \\ x_{d-1} &= r \sin\theta_{d-2} \cos\theta_{d-3}, \\ x_d &= r \cos\theta_{d-2}, \end{aligned}$$

be the spherical coordinates in d dimensions with $r = \sqrt{x_1^2 + x_2^2 + \ldots + x_d^2}$, $0 \le \theta_i \le \pi$, for all $i = 1, 2, \ldots, d-2$ and $0 \le \phi \le 2\pi$, then the Jacobian is given by

$$\det\left(\frac{\partial(x_1, x_2, \ldots, x_d)}{\partial(r, \theta_1, \ldots, \theta_{d-2}, \phi)}\right) = r^{d-1} \sin^{d-2}(\theta_1) \sin^{d-3}(\theta_2) \ldots \sin^2(\theta_{d-3}) \sin(\theta_{d-2}). \tag{6.3}$$

Definition 6.1.3 *The Laplace operator Δ_d in $\mathbb{R}^d$ is given as*

$$\Delta_d := \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \ldots + \frac{\partial^2}{\partial x_d^2}.$$

In terms of spherical coordinates, it takes the following representation:

$$\Delta_d := r^{1-d} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} + \frac{1}{r^2} \Delta^*_{\xi_d}, \tag{6.4}$$

where $\Delta^*_{\xi_d}$ denotes the Laplace-Beltrami operator of the unit sphere Ω^{d-1} and is defined as

$$\begin{aligned} \Delta^*_{\xi_d} &= (1-t^2)\frac{\partial^2}{\partial t^2} - (d-1)t\frac{\partial}{\partial t} + \frac{1}{1-t^2}\Delta^*_{\xi_{d-1}}, \quad d \ge 3, \\ \Delta^*_{\xi_2} &= \frac{\partial^2}{\partial \phi^2}. \end{aligned}$$

Definition 6.1.4 *The function $P_n^d(\cdot) : t \mapsto P_n^d(t)$ for $t \in [-1, 1]$ and $n \in \mathbb{N}_0$ is called the Legendre polynomial of degree n and dimension d and is determined by the following properties:*

(i) P_n^d is a polynomial with degree n.

(ii) For $n,\, m \in \mathbb{N}_0$,

$$\int_{-1}^{1} P_n^d(t) P_m^d(t)(1-t^2)^{\frac{d-3}{2}} \mathrm{d}t = 0, \quad \textit{if } n \neq m.$$

(iii) $P_n^d(1) = 1$.

Remark 6.1.5 *The Legendre polynomials $P_n^d(t)$ can be defined in terms of Gegenbauer polynomials, i.e.*

$$P_n^d(t) = \frac{\Gamma(d-2)\Gamma(n+1)}{\Gamma(d-2+n)} C_n^{\frac{d}{2}-1}(t), \quad t \in [-1,1]. \tag{6.5}$$

The recurrence relation for the Legendre polynomials $P_n^d(t)$ directly follows from the recurrence relation of Gegenbauer polynomials. With $\lambda = \frac{d}{2} - 1$, (1.37) yields

$$nC_n^{\frac{d}{2}-1}(t) = 2\left(n + \frac{d}{2} - 2\right) t\, C_{n-1}^{\frac{d}{2}-1}(t) - (n+d-4) C_{n-2}^{\frac{d}{2}-1}(t). \tag{6.6}$$

With the help of (6.5), we obtain

$$\begin{aligned} &\frac{\Gamma(d-2+n)}{\Gamma(d-2)\Gamma(n+1)}\, nP_n^d(t) \\ &= 2\left(n+\frac{d}{2}-2\right)\frac{\Gamma(d-3+n)}{\Gamma(d-2)\Gamma(n)}\, t\, P_{n-1}^d(t) - \frac{(n+d-4)\Gamma(d-4+n)}{\Gamma(d-2)\Gamma(n-1)}\, P_{n-2}^d(t). \end{aligned}$$

Further, an easy simplification gives

$$(n+d-3)P_n^d(t) = (2n+d-4)t\, P_{n-1}^d(t) - (n-1)P_{n-2}^d(t), \quad n \geq 2, \tag{6.7}$$

where $P_0^d(t) = 1$ and $P_1^d(t) = t$.

6.2 Spherical Harmonics in d Dimensions

In this section, we introduce the spherical harmonics in d dimensions and also provide their properties that will be required later. For details the reader is referred to [19] and [53].

Definition 6.2.1 *A polynomial H_n in $\mathbb{R}^d$ is called a harmonic homogeneous polynomial of degree n in d variables if the following two conditions hold:*

$$H_n(tx_1, tx_2, \ldots, tx_d) = t^n H_n(x_1, x_2, \ldots, x_d), \quad t \in \mathbb{R},$$

and

$$\Delta_d H_n(x_1, x_2, \ldots, x_d) = 0.$$

Theorem 6.2.2 *Let $\mathcal{Z}(d,n)$ represent the maximum number of linearly independent homogeneous harmonic polynomials in $\mathbb{R}^d$ of degree n, then*

$$\mathcal{Z}(d,n) = \frac{(2n+d-2)(n+d-3)!}{(d-2)!\,n!}. \tag{6.8}$$

Following Definition 1.3.5, spherical harmonics Y_n^d of degree n in d variables are harmonic homogeneous polynomials H_n, restricted to the $(d-1)$-sphere, i.e. $Y_n^d = H_n|_{\Omega^{d-1}}$. The space of all spherical harmonics of degree n in d variables is denoted by $\mathrm{Harm}_n(\Omega^{d-1})$.

Theorem 6.2.3 *For all $d \geq 3$ and $n \in \mathbb{N}_0$, the dimension of the space $\mathrm{Harm}_n(\Omega^{d-1})$ is given by*

$$\dim\big(\mathrm{Harm}_n(\Omega^{d-1})\big) = \mathcal{Z}(d,n). \tag{6.9}$$

Theorem 6.2.4 *Spherical harmonics are the eigenfunctions of the Laplace-Beltrami operator $\Delta^*_{\xi_d}$ corresponding to the eigenvalues $-n(n+d-2)$, i.e.*

$$\Delta^*_{\xi_d} Y_n^d(\xi) = -n(n+d-2) Y_n^d(\xi). \tag{6.10}$$

Proof: The decomposition of H_n into its radial and angular parts is given as

$$H_n(r\xi) = r^n Y_n^d(\xi).$$

Calculating the Laplacian of the above equation with the help of (6.4), we obtain

$$\begin{aligned}
\Delta_d H_n(r\xi) &= \Delta_d\left(r^n Y_n^d(\xi)\right), \quad r>0,\ \xi\in\Omega \\
\Leftrightarrow \quad 0 &= \left(\frac{\partial^2}{\partial r^2} + \frac{d-1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta^*_{\xi_d}\right) r^n Y_n^d(\xi) \quad r>0,\ \xi\in\Omega \\
\Leftrightarrow \quad 0 &= \left(n(n-1) + n(d-1) + \Delta^*_{\xi_d}\right) r^{n-2} Y_n^d(\xi) \quad r>0,\ \xi\in\Omega \\
\Leftrightarrow \quad 0 &= \left(n(n-1) + n(d-1) + \Delta^*_{\xi_d}\right) Y_n^d(\xi), \quad \xi\in\Omega \\
\Leftrightarrow \Delta^*_{\xi_d} Y_n^d(\xi) &= -n(n+d-2) Y_n^d(\xi), \quad \xi\in\Omega.
\end{aligned}$$

■

Theorem 6.2.5 *Spherical harmonics Y_n^d satisfy the following property:*

$$\left|Y_n^d(\xi)\right| \leq \sqrt{\frac{\mathcal{Z}(d,n)}{\omega_d}\int_{\Omega^{d-1}} \left(Y_n^d(\eta)\right)^2 \mathrm{d}\omega(\eta)} \ \textit{for all}\ \xi\in\Omega. \tag{6.11}$$

Theorem 6.2.6 *Spherical harmonics Y_n^d and Y_m^d of degrees $n, m \in \mathbb{N}_0$, with $n \neq m$, are orthogonal with respect to the $\mathrm{L}^2(\Omega^{d-1})$-inner product, i.e.*

$$\int_{\Omega^{d-1}} Y_n^d(\xi) Y_m^d(\xi)\, \mathrm{d}\omega(\xi) = 0. \tag{6.12}$$

Definition 6.2.7 *The system $\{Y_{n,j}^d\}_{j=1,2,\ldots,\mathcal{Z}(d,n)}$ for every fixed $n \in \mathbb{N}_0$ represents an orthonormal system in $\mathrm{Harm}_n(\Omega^{d-1})$, i.e.*

$$\int_{\Omega^{d-1}} Y_{n,j}^d(\xi) Y_{n,k}^d(\xi)\, \mathrm{d}\omega(\xi) = \delta_{jk}, \quad j,k \in \{1,2,\ldots,\mathcal{Z}(d,n)\}. \tag{6.13}$$

In accordance with Theorem 6.2.3, the set $\{Y_{n,j}^d\}$ for $j = 1,2,\ldots,\mathcal{Z}(d,n)$ is a maximal linearly independent set of spherical harmonics and hence configures a complete orthonormal system in $\left(\mathrm{Harm}_n(\Omega^{d-1}), \langle\cdot,\cdot\rangle_{\mathrm{L}^2(\Omega^{d-1})}\right)$, i.e. for $F \in \mathrm{Harm}_n\left(\Omega^{d-1}\right)$,

$$\left\langle F, Y_{n,j}^d \right\rangle_{\mathrm{L}^2(\Omega^{d-1})} = 0 \text{ for all } j \in \{1,2,\ldots,\mathcal{Z}(d,n)\} \text{ implies } F = 0 \tag{6.14}$$

and

$$\int_{\Omega^{d-1}} Y_{n,j}^d(\xi) Y_{m,k}^d(\xi)\, \mathrm{d}\omega(\xi) = \delta_{nm}\delta_{jk}, \quad j,k \in \{1,2,\ldots,\mathcal{Z}(d,n)\}. \tag{6.15}$$

The succeeding theorem is an immediate consequence of previous considerations, that are: Theorem 6.2.6, Definition 6.2.7 and equation (6.9).

Theorem 6.2.8 *For n, $m \in \mathbb{N}_0$, the system $\{Y_{n,j}^d\}_{j=1,2,\ldots,\mathcal{Z}(d,n)}$ denotes an orthonormal basis in $\left(\mathrm{Harm}_n(\Omega^{d-1}), \langle\cdot,\cdot\rangle_{\mathrm{L}^2(\Omega^{d-1})}\right)$.*

Moreover, the system $\{Y_{n,j}^d\}_{n\in\mathbb{N}_0; j=1,2,\ldots,\mathcal{Z}(d,n)}$ represents a complete orthonormal system in the Hilbert space $(\mathrm{L}^2(\Omega^{d-1}), \langle\cdot,\cdot\rangle_{\mathrm{L}^2(\Omega^{d-1})})$. Further, we state the addition theorem for higher dimensions (see [53]).

Theorem 6.2.9 *For an orthonormal basis system $\{Y_{n,j}^d\}_{n\in\mathbb{N}_0; j=1,2,\ldots,\mathcal{Z}(d,n)}$ and the Legendre polynomials P_n^d in d dimensions, the following relation exists:*

$$\sum_{j=1}^{\mathcal{Z}(d,n)} Y_{n,j}^d(\xi) Y_{n,j}^d(\eta) = \frac{\mathcal{Z}(d,n)}{\omega_d} P_n^d(\xi\cdot\eta), \quad \xi,\eta \in \Omega^{d-1}, \tag{6.16}$$

where ω_d is the surface area of the sphere Ω^{d-1}.

6.3 Orthonormal Systems in d Dimensions

In this section, we construct a complete orthonormal system for the space $\mathrm{L}^2(\mathcal{B}_R^d)$. In order to achieve this objective, we follow the separation approach. A similar approach for the 3-dimensional case can be found in [47].
We consider a function $G^d \in \mathrm{L}^2(\mathcal{B}_R^d)$ with a representation of the form such that the radial and the angular parts of the function can be separated, i.e.

$$G^d(x) = F^d(|x|)\, Y^d\left(\frac{x}{|x|}\right), \quad x \in \mathcal{B}_R^d \setminus \{0\}.$$

Then, for $\tilde{G}^d \in \mathrm{L}^2(\mathcal{B}_R^d)$ with

$$\tilde{G}^d(x) = \tilde{F}^d(|x|)\, \tilde{Y}^d\left(\frac{x}{|x|}\right), \quad x \in \mathcal{B}_R^d \setminus \{0\},$$

the inner product of G^d with $\tilde{G}^d$ in $\mathrm{L}^2(\mathcal{B}_R^d)$ is given by

$$\begin{aligned}\left\langle G^d, \tilde{G}^d \right\rangle_{\mathrm{L}^2\left(\mathcal{B}_R^d\right)} &= \int_{\mathcal{B}_R^d} G^d(x)\tilde{G}^d(x)\,\mathrm{d}x \\ &= \int_0^R r^{d-1} F^d(r)\tilde{F}^d(r)\,\mathrm{d}r \int_{\Omega^{d-1}} Y^d(\xi)\tilde{Y}^d(\xi)\,\mathrm{d}\omega(\xi).\end{aligned}$$

Now, we have to choose the radial part F^d and the angular part Y^d of the function such that they are orthonormal in the L^2-space. From the above integral equation, it is easy to see that we can choose $Y^d(\xi) = Y_{n,j}^d(\xi)$, which forms an orthonormal system in $\mathrm{L}^2\left(\Omega^{d-1}\right)$ (see Section 6.2). Now, we denote the function G^d by $G_{\alpha,n,j}^d$, with an unknown index α for the radial part F^d and the indices n, j representing the angular part, i.e. the degree and the order of the d-dimensional spherical harmonics, respectively as follows:

$$G_{\alpha,n,j}^d(x) = F_\alpha^d(|x|)\, Y_{n,j}^d\left(\frac{x}{|x|}\right), \; x \in \mathcal{B}_R^d \setminus \{0\},$$

where $n \in \mathbb{N}_0$ and $j = 1, 2, \ldots, \mathcal{Z}(d, n)$. Now, we are left with the unknown function F^d with index α. Next, in order to have a complete system $G_{\alpha,n,j}^d$ in $\mathrm{L}^2(\mathcal{B}_R^d)$, we consider for a function $f \in \mathrm{L}^2\left(\mathcal{B}_R^d\right)$,

$$\left\langle f, G_{\alpha,n,j}^d \right\rangle_{\mathrm{L}^2(\mathcal{B}_R^d)} = 0 \; \text{ for all } \alpha, n, j.$$

Then,

$$\begin{aligned}0 &= \int_{\mathcal{B}_R^d} f(x) G_{\alpha,n,j}^d(x)\mathrm{d}x \\ &= \int_{\Omega^{d-1}} Y_{n,j}^d(\xi) \int_0^R r^{d-1} F_\alpha^d(r) f(r\xi)\,\mathrm{d}r\,\mathrm{d}\omega(\xi).\end{aligned}$$

Since $\left\{Y_{n,j}^d\right\}_{n\in\mathbb{N}_0;j=1,2,\ldots,\mathcal{Z}(d,n)}$ is complete in the space $\mathrm{L}^2(\Omega^{d-1})$, we are left with the following equation:

$$\int_0^R r^{d-1}F_\alpha^d(r)f(r\xi)\mathrm{d}r = 0$$

for almost every $\xi \in \Omega^{d-1}$. This shows that the system $G_{\alpha,n,j}^d$ can be complete in $\mathrm{L}^2(\mathcal{B}_R^d)$ only if F_α^d is complete in the space $\mathrm{L}_w^2[0,R]$ with weights $w(r) = r^{d-1}$. As proposed in [4, 47, 72] for the 3-dimensional case, we can either choose F_α^d such that apart from its radial dependence, it also depends on the degree n of the angular part, i.e. for $r \in \mathbb{R}_0^+$

$$F_\alpha^{\mathrm{I},d}(r) := r^{l_n}\tilde{F}_{m,n}^{\mathrm{I},d}(r^2), \quad n, m \in \mathbb{N}_0. \tag{6.17}$$

Here, we also consider the case from [50], i.e. r^{l_n}, where $l_n \geq -1$ for all $n \in \mathbb{N}_0$. Then we have,

$$G_{m,n,j}^{\mathrm{I},d}(r\xi) = r^{l_n}\tilde{F}_{m,n}^{\mathrm{I},d}(r^2)Y_{n,j}^d(\xi) \tag{6.18}$$

or we can set F_α^d such that it only has the radial dependency, i.e. for $r \in \mathbb{R}_0^+$

$$F_\alpha^{\mathrm{II},d}(r) = F_m^{\mathrm{II},d}(r), \quad m \in \mathbb{N}_0. \tag{6.19}$$

So, the system of functions in this case is given by

$$G_{m,n,j}^{\mathrm{II},d}(r\xi) = F_m^{\mathrm{II},d}(r)Y_{n,j}^d(\xi). \tag{6.20}$$

These systems have their advantages and disadvantages. The system of type I with $l_n = n$ yields an algebraic polynomial in $x_1, x_2, \ldots, x_d$. The second choice of system has an advantage over the first one, as it completely decouples the angular and radial parts of the system but also has a disadvantage of being discontinuous in $x = 0$.

We now consider the inner product of our first choice of function F_α^d given by (6.17) in $\mathrm{L}_w^2[0,R]$ with weights r^{d-1} as follows

$$\begin{aligned}\delta_{m_1,m_2} &= \int_0^R r^{d-1}r^{l_n}\tilde{F}_{m_1,n}^{\mathrm{I},d}(r^2)r^{l_n}\tilde{F}_{m_2,n}^{\mathrm{I},d}(r^2)\,\mathrm{d}r\\ &= \int_0^R r^{2l_n+d-1}\tilde{F}_{m_1,n}^{\mathrm{I},d}(r^2)\tilde{F}_{m_2,n}^{\mathrm{I},d}(r^2)\,\mathrm{d}r.\end{aligned}$$

Substituting

$$r = R\sqrt{\frac{t+1}{2}},$$

we get

$$\begin{aligned}
&\delta_{m_1,m_2}\\
&= \int_{-1}^{1} \left(R^2 \frac{t+1}{2}\right)^{l_n+\frac{d-1}{2}} \tilde{F}^{\mathrm{I},d}_{m_1,n}\left(R^2\frac{t+1}{2}\right) \tilde{F}^{\mathrm{I},d}_{m_2,n}\left(R^2\frac{t+1}{2}\right) \frac{R\mathrm{d}t}{\sqrt{8(t+1)}}\\
&= \frac{R^{2l_n+d}}{2^{l_n+\frac{d}{2}+1}} \int_{-1}^{1} (1+t)^{l_n+\frac{d}{2}-1} \tilde{F}^{\mathrm{I},d}_{m_1,n}\left(R^2\frac{t+1}{2}\right) \tilde{F}^{\mathrm{I},d}_{m_2,n}\left(R^2\frac{t+1}{2}\right) \mathrm{d}t.
\end{aligned}$$

The above equation implies that our required functions are the Jacobi polynomials (Definition 1.2.1) orthogonal in the space $\mathrm{L}^2_w[-1,1]$ with weights $(1-t)^0(1+t)^{l_n+\frac{d}{2}-1}$ and $t = 2\frac{r^2}{R^2} - 1$. Thus, we obtain

$$\tilde{F}^{\mathrm{I},d}_{m,n}(r^2) = a_{m,n} P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2} - 1\right), \quad r \in \mathbb{R}^+_0.$$

Since the polynomials $\tilde{F}^{\mathrm{I},d}_{m,n}$ should be orthonormal, using the requirement of having norm 1, we can determine the constant $a_{m,n}$, i.e.

$$1 = \frac{R^{2l_n+d}}{2^{l_n+\frac{d}{2}+1}}\, a^2_{m,n} \int_{-1}^{1} (1+t)^{l_n+\frac{d}{2}-1} \left(P_m^{(0,l_n+\frac{d}{2}-1)}(t)\right)^2 \mathrm{d}t.$$

Using Theorem 1.2.11 and simplifying, we arrive at

$$\begin{aligned}
1 &= \frac{R^{2l_n+d}}{2^{l_n+\frac{d}{2}+1}}\, a^2_{m,n}\, \frac{2^{l_n+\frac{d}{2}}}{2m+l_n+\frac{d}{2}} \cdot \frac{\Gamma(m+1)\Gamma(m+l_n+\frac{d}{2})}{m!\,\Gamma(m+l_n+\frac{d}{2})}\\
\frac{4m+2l_n+d}{R^{2l_n+d}} &= a^2_{m,n}.
\end{aligned}$$

This results in the following choice of a complete orthonormal system:

$$G^{\mathrm{I},d}_{m,n,j}(r\xi) = \sqrt{\frac{4m+2l_n+d}{R^d}} \left(\frac{r}{R}\right)^{l_n} P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2} - 1\right) Y^d_{n,j}(\xi). \quad (6.21)$$

Constructing the second system in the same way, we now take the second function given by (6.19). In order to have an orthogonal function $F^{\mathrm{II},d}_m$, we need to proceed (similarly as above) in the following way:

$$\delta_{m_1,m_2} = \int_0^R r^{d-1} F^{\mathrm{II},d}_{m_1}(r) F^{\mathrm{II},d}_{m_2}(r)\, \mathrm{d}r.$$

We substitute

$$r = R\,\frac{t+1}{2},$$

in the above equation and get

$$\begin{aligned}\delta_{m_1,m_2} &= \int_{-1}^{1} \left(R\frac{t+1}{2}\right)^{d-1} F_{m_1}^{\mathrm{II},d}\left(R\frac{t+1}{2}\right) F_{m_2}^{\mathrm{II},d}\left(R\frac{t+1}{2}\right)\frac{R}{2}\mathrm{d}t \\ &= \left(\frac{R}{2}\right)^{d} \int_{-1}^{1} (1+t)^{d-1} F_{m_1}^{\mathrm{II},d}\left(R\frac{t+1}{2}\right) F_{m_2}^{\mathrm{II},d}\left(R\frac{t+1}{2}\right)\mathrm{d}t.\end{aligned}$$

Our required functions in this case are the Jacobi polynomials with weights $(1-t)^0(1+t)^{d-1}$, hence, we have

$$F_m^{\mathrm{II},d}(r) = b_m P_m^{(0,d-1)}\left(2\frac{r}{R}-1\right).$$

In order to find the constant b_m, we proceed likewise as before. Using Theorem 1.2.11, we have

$$\begin{aligned}1 &= \left(\frac{R}{2}\right)^{d} b_m^2 \int_{-1}^{1} (1+t)^{d-1} \left(P_m^{(0,d-1)}(t)\right)^2 \mathrm{d}t \\ 1 &= \frac{R^d}{2m+d} b_m^2,\end{aligned}$$

which finally gives us a choice of second complete orthonormal system in $\mathrm{L}^2\left(\mathcal{B}_R^d\right)$, i.e.

$$G_{m,n,j}^{\mathrm{II},d}(r\xi) = \sqrt{\frac{2m+d}{R^d}} P_m^{(0,d-1)}\left(2\frac{r}{R}-1\right) Y_{n,j}^d(\xi). \tag{6.22}$$

This helps us to formulate the following result.

Theorem 6.3.1 *The systems of functions* $\{G_{m,n,j}^{\mathrm{X},d}\}_{m,n\in\mathbb{N}_0;j=1,\ldots,\mathcal{Z}(d,n)}$ *defined by* (6.21) *for* X = I *and by* (6.22) *for* X = II *respectively, form complete orthonormal systems in* $\mathrm{L}^2(\mathcal{B}_R^d)$.

6.4 Differential Operators for Orthonormal Systems on $\mathcal{B}_R^d$

This section introduces a class of differential operators for the orthonormal systems of types I and II given by (6.21) and (6.22) respectively, such that these orthonormal systems form eigenfunctions for these operators. Analogous calculations have been done for the dimension $d = 3$ in [2] and [50]. From (6.21) and (6.22), we can see that our orthonormal systems of types I and II are comprised of Jacobi polynomials and spherical harmonics. So, in order to calculate their differential operators, we begin with calculating the operators for Jacobi polynomials and spherical harmonics. The following result, for the spherical harmonics in d variables, is borrowed from [32].

Theorem 6.4.1 *Spherical harmonics $Y^d_{n,j}$, for $n \in \mathbb{N}_0$, $j \in \{1, 2, \ldots, \mathcal{Z}(d, n)\}$ form the eigenfunctions of the invertible differential operator $\left(-\Delta^*_{\xi_d} + (\frac{d-2}{2})^2\right)$, i.e.*

$$\left(-\Delta^*_{\xi_d} + \left(\frac{d-2}{2}\right)^2\right) Y^d_{n,j} = \left(n + \frac{d-2}{2}\right)^2 Y^d_{n,j}, \tag{6.23}$$

where $\Delta^*_{\xi_d}$ is the Beltrami operator. In general, for $\ell \in \mathbb{N}$

$$\left(-\Delta^*_{\xi_d} + \left(\frac{d-2}{2}\right)^2\right)^\ell Y^d_{n,j} = \left(n + \frac{d-2}{2}\right)^{2\ell} Y^d_{n,j}. \tag{6.24}$$

Proof: From equation (6.10), we have

$$-\Delta^*_{\xi_d} Y^d_n(\xi) = n(n + d - 2) Y^d_n(\xi).$$

Thus, for the operator $\left(-\Delta^*_{\xi_d} + (\frac{d-2}{2})^2\right)$, we obtain

$$\begin{aligned}
\left(-\Delta^*_{\xi_d} + \left(\frac{d-2}{2}\right)^2\right) Y^d_{n,j} &= -\Delta^*_{\xi_d} Y^d_{n,j} + \left(\frac{d-2}{2}\right)^2 Y^d_{n,j} \\
&= n(n + d - 2) Y^d_{n,j} + \left(\frac{d-2}{2}\right)^2 Y^d_{n,j} \\
&= \left(n^2 + (d-2)n + \frac{(d-2)^2}{4}\right) Y^d_{n,j} \\
&= \left(n + \frac{d-2}{2}\right)^2 Y^d_{n,j}.
\end{aligned}$$

By induction, we obtain the general case for $\ell \in \mathbb{N}$. ■

Next, we derive the differential operator for Jacobi polynomials with particular value of parameters. From Theorem 1.2.3, the differential equation for $P_m^{(0,l_n+\frac{d}{2}-1)}$ with parameters $\alpha = 0$ and $\beta = l_n + \frac{d}{2} - 1$ is given by

$$\begin{aligned}
\left(1 - y^2\right) \frac{\mathrm{d}^2}{\mathrm{d}y^2} P_m^{(0,l_n+\frac{d}{2}-1)}(y) + \left(l_n + \frac{d}{2} - 1 - \left(l_n + \frac{d}{2} + 1\right) y\right) \frac{\mathrm{d}}{\mathrm{d}y} P_m^{(0,l_n+\frac{d}{2}-1)}(y) \\
+ m \left(m + l_n + \frac{d}{2}\right) P_m^{(0,l_n+\frac{d}{2}-1)}(y) = 0.
\end{aligned}$$

Substituting $y = 2\frac{r^2}{R^2} - 1$, i.e. $r = R\sqrt{\frac{y+1}{2}}$ with $\frac{\mathrm{d}r}{\mathrm{d}y} = \frac{R^2}{4r}$, we get

$$\left(1 - \left(2\frac{r^2}{R^2} - 1\right)^2\right) \frac{\mathrm{d}^2}{\mathrm{d}y^2} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right)$$
$$+ \left(l_n + \frac{d}{2} - 1 - \left(l_n + \frac{d}{2} + 1\right)\left(2\frac{r^2}{R^2} - 1\right)\right) \frac{\mathrm{d}}{\mathrm{d}y} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right)$$
$$+ m\left(m + l_n + \frac{d}{2}\right) P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right) = 0. \quad (6.25)$$

Now, differentiating $P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2} - 1\right)$ with respect to y using the chain rule, we have

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}y} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right) &= \frac{\mathrm{d}}{\mathrm{d}r} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right) \frac{\mathrm{d}r}{\mathrm{d}y} \\ &= \frac{\mathrm{d}}{\mathrm{d}r} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right) \frac{R^2}{4r}. \end{aligned} \quad (6.26)$$

Again differentiating with respect to y, we obtain

$$\begin{aligned} &\frac{\mathrm{d}^2}{\mathrm{d}y^2} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right) \\ &= \frac{\mathrm{d}^2}{\mathrm{d}r^2} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right) \frac{R^4}{16r^2} - \frac{\mathrm{d}}{\mathrm{d}r} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right) \frac{R^4}{16r^3}. \end{aligned} \quad (6.27)$$

In order to avoid any confusion in calculations, we simplify equation (6.25) in parts. At first, we consider the first term in (6.25). Inserting the second derivative of $P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2} - 1\right)$ from (6.27), we get

$$\begin{aligned} &\left(1 - \left(2\frac{r^2}{R^2} - 1\right)^2\right) \frac{\mathrm{d}^2}{\mathrm{d}y^2} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right) \\ &= \left(\frac{4r^2}{R^2} - \frac{4r^4}{R^4}\right) \frac{R^4}{16r^2} \frac{\mathrm{d}^2}{\mathrm{d}r^2} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right) \\ &\quad - \left(\frac{4r^2}{R^2} - \frac{4r^4}{R^4}\right) \frac{R^4}{16r^3} \frac{\mathrm{d}}{\mathrm{d}r} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right) \\ &= \left(\frac{R^2 - r^2}{4}\right) \frac{\mathrm{d}^2}{\mathrm{d}r^2} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right) \\ &\quad - \left(\frac{R^2 - r^2}{4r}\right) \frac{\mathrm{d}}{\mathrm{d}r} P_m^{(0,l_n+\frac{d}{2}-1)} \left(2\frac{r^2}{R^2} - 1\right). \end{aligned} \quad (6.28)$$

Next, simplifying the second term of (6.25) with the help of equation (6.26), we have

$$\begin{aligned}
&\left(l_n+\frac{d}{2}-1-\left(l_n+\frac{d}{2}+1\right)\left(2\frac{r^2}{R^2}-1\right)\right)\frac{\mathrm{d}}{\mathrm{d}y}P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right)\\
&=\left(l_n+\frac{d}{2}-1-\left(l_n+\frac{d}{2}+1\right)\left(2\frac{r^2}{R^2}-1\right)\right)\frac{R^2}{4r}\frac{\mathrm{d}}{\mathrm{d}r}P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right)\\
&=\left(2l_n+d-\left(l_n+\frac{d}{2}+1\right)2\frac{r^2}{R^2}\right)\frac{R^2}{4r}\frac{\mathrm{d}}{\mathrm{d}r}P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right).
\end{aligned}\tag{6.29}$$

If we use the values from equations (6.28) and (6.29), (6.25) yields

$$\begin{aligned}
&\left(R^2-r^2\right)\frac{\mathrm{d}^2}{\mathrm{d}r^2}P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right)+\left((2l_n+d-1)-(2l_n+d+1)\frac{r^2}{R^2}\right)\frac{R^2}{r}\\
&\times\frac{\mathrm{d}}{\mathrm{d}r}P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right)+4m\left(m+l_n+\frac{d}{2}\right)P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right)=0,
\end{aligned}$$

which results in the following equation:

$$\begin{aligned}
&\left(\left(R^2-r^2\right)\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\left((2l_n+d-1)-(2l_n+d+1)\frac{r^2}{R^2}\right)\frac{R^2}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)\\
&\times P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right)=-4m\left(m+l_n+\frac{d}{2}\right)P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right).
\end{aligned}\tag{6.30}$$

Now, we define new functions $p(r):=P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right)$ and $g(r):=p(r)\left(\frac{r}{R}\right)^{l_n}$. The first and second derivatives of the function g are

$$\begin{aligned}
g'(r)&=p'(r)\left(\frac{r}{R}\right)^{l_n}+p(r)\frac{l_n}{R}\left(\frac{r}{R}\right)^{l_n-1}\\
&=p'(r)\left(\frac{r}{R}\right)^{l_n}+g(r)\frac{l_n}{r}
\end{aligned}$$

and

$$\begin{aligned}
g''(r)&=p''(r)\left(\frac{r}{R}\right)^{l_n}+p'(r)\frac{l_n}{R}\left(\frac{r}{R}\right)^{l_n-1}+g'(r)\frac{l_n}{r}-g(r)\frac{l_n}{r^2}\\
&=p''(r)\left(\frac{r}{R}\right)^{l_n}+2g'(r)\frac{l_n}{r}-g(r)\frac{l_n(l_n+1)}{r^2},
\end{aligned}$$

respectively. Multiplying the above equation by the term $(R^2 - r^2)$ and substituting the value of $(R^2 - r^2)p''$ from equation (6.30), we get

$$\left(R^2 - r^2\right) g'' = -\left((2l_n + d - 1) - (2l_n + d + 1)\frac{r^2}{R^2}\right) \frac{R^2}{r} \left(\frac{r}{R}\right)^{l_n} p'$$
$$- 4m\left(m + l_n + \frac{d}{2}\right)\left(\frac{r}{R}\right)^{l_n} p + 2(R^2 - r^2)g' \frac{l_n}{r} - (R^2 - r^2)g \frac{l_n(l_n + 1)}{r^2}.$$

Further, simplifying the equation using the values of p and p', we get

$$\begin{aligned}\left(R^2 - r^2\right) g'' = &-\left((2l_n + d - 1) - (2l_n + d + 1)\frac{r^2}{R^2}\right) \frac{R^2}{r}\left(g' - \frac{l_n}{r} g\right) \\ &- 4m\left(m + l_n + \frac{d}{2}\right) g + 2\left(R^2 - r^2\right) g' \frac{l_n}{r} - \left(R^2 - r^2\right) g \frac{l_n(l_n + 1)}{r^2} \\ = &\left(2\frac{l_n}{r}\left(R^2 - r^2\right) - (2l_n + d - 1)\frac{R^2}{r} + (2l_n + d + 1)r\right) g' \\ &+ \left((2l_n + d - 1)\frac{R^2 l_n}{r^2} - (2l_n + d + 1)l_n - \frac{(R^2 - r^2)}{r^2} l_n(l_n + 1)\right. \\ &\left. - 4m\left(m + l_n + \frac{d}{2}\right) g\right).\end{aligned}$$

Consequently, we have

$$\begin{aligned}\left(R^2 - r^2\right) g'' - \left((d + 1)r - (d - 1)\frac{R^2}{r}\right) g' - \left((l_n + d - 2)l_n \frac{R^2}{r^2}\right) g& \\ = -\left(l_n(l_n + d) + 4m\left(m + l_n + \frac{d}{2}\right)\right) g.&\end{aligned}$$

This gives us the differential operator for $g(r) = \left(\frac{r}{R}\right)^{l_n} P_m^{(0, l_n + \frac{d}{2} - 1)}\left(2\frac{r^2}{R^2} - 1\right)$ corresponding to the eigenvalues $\left(-l_n(l_n + d) - 4m(m + l_n + \frac{d}{2})\right)$. A similar procedure can be followed to find the differential operator of Jacobi polynomials $P_m^{(0,d-1)}\left(2\frac{r}{R} - 1\right)$ with parameters $\alpha = 0$ and $\beta = d-1$. The differential equation corresponding to the given parameters is given by

$$\left(1 - y^2\right) \frac{\mathrm{d}^2}{\mathrm{d}y^2} P_m^{(0,d-1)}(y) + (d - 1 - (d + 1)y) \frac{\mathrm{d}}{\mathrm{d}y} P_m^{(0,d-1)}(y) + m(m + d) P_m^{(0,d-1)}(y) = 0.$$

Further, substituting $y = 2\frac{r}{R} - 1$ and simplifying, we get

$$\begin{aligned}r(R - r)\frac{\mathrm{d}^2}{\mathrm{d}r^2} P_m^{(0,d-1)}\left(2\frac{r}{R} - 1\right) + \left(2d - 2(d + 1)\frac{r}{R}\right) \frac{R}{2} \frac{\mathrm{d}}{\mathrm{d}r} P_m^{(0,d-1)}\left(2\frac{r}{R} - 1\right)& \\ + m(m + d) P_m^{(0,d-1)}\left(2\frac{r}{R} - 1\right) = 0.&\end{aligned}$$

This results in the following equation:

$$\left(r(R-r)\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\left(2d-2(d+1)\frac{r}{R}\right)\frac{R}{2}\frac{\mathrm{d}}{\mathrm{d}r}\right)P_m^{(0,d-1)}\left(2\frac{r}{R}-1\right)$$
$$=-m(m+d)P_m^{(0,d-1)}\left(2\frac{r}{R}-1\right).$$

This enables us to state the next theorem.

Theorem 6.4.2 *For $n,m\in\mathbb{N}_0$ and $l_n\geq -1$, $P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}$ forms an eigenfunction of the differential operator*

$$D^{\mathrm{I}_d}=\left(R^2-r^2\right)\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\left((d+1)r-(d-1)\frac{R^2}{r}\right)\frac{\mathrm{d}}{\mathrm{d}r}-\left((l_n+d-2)l_n\frac{R^2}{r^2}\right),$$

corresponding to the eigenvalues

$$\left(D^{\mathrm{I}_d}\right)^\wedge(m,n)=-\left(l_n(l_n+d)+4m\left(m+l_n+\frac{d}{2}\right)\right)$$

and $P_m^{(0,d-1)}\left(2\frac{r}{R}-1\right)$ are eigenfunctions for the differential operator

$$D^{\mathrm{II}_d}=r(R-r)\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\left(2d-2(d+1)\frac{r}{R}\right)\frac{R}{2}\frac{\mathrm{d}}{\mathrm{d}r},$$

corresponding to the eigenvalues

$$\left(D^{\mathrm{II}_d}\right)^\wedge(m)=-m(m+d).$$

In addition to this, we can now derive the invertible differential operators for $P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}$ and $P_m^{(0,d-1)}\left(2\frac{r}{R}-1\right)$.

Theorem 6.4.3 *For $\mathrm{X}\in\{\mathrm{I},\mathrm{II}\}$, the differential operators $\left(-D^{\mathrm{X}_d}+\frac{d^2}{4}\right)^\ell$, $\ell\in\mathbb{N}$ are invertible differential operators and their eigenvalues corresponding to the eigenfunctions $P_m^{(0,l_n+\frac{d}{2}-1)}\left(2\frac{r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}$ and $P_m^{(0,d-1)}\left(2\frac{r}{R}-1\right)$ respectively, are $\left(l_n+2m+\frac{d}{2}\right)^{2\ell}$ and $\left(m+\frac{d}{2}\right)^{2\ell}$.*

Proof: We begin the proof with the type I operator.

$$\left(-D^{\mathrm{I}_d}+\frac{d^2}{4}\right)\left(P_m^{(0,l_n+\frac{d}{2}-1)}\left(\frac{2r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}\right)$$
$$=-D^{\mathrm{I}_d}\left(P_m^{(0,l_n+\frac{d}{2}-1)}\left(\frac{2r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}\right)$$
$$+\frac{d^2}{4}\left(P_m^{(0,l_n+\frac{d}{2}-1)}\left(\frac{2r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}\right).$$

According to Theorem 6.4.2, for $\ell = 1$, we have

$$\begin{aligned}
&\left(-D^{\mathrm{I}_d} + \frac{d^2}{4}\right)\left(P_m^{(0,l_n+\frac{d}{2}-1)}\left(\frac{2r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}\right)\\
&= \left(l_n(l_n+d) + 4m\left(m + l_n + \frac{d}{2}\right) + \frac{d^2}{4}\right)\left(P_m^{(0,l_n+\frac{d}{2}-1)}\left(\frac{2r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}\right)\\
&= \left(l_n + 2m + \frac{d}{2}\right)^2\left(P_m^{(0,l_n+\frac{d}{2}-1)}\left(\frac{2r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}\right).
\end{aligned}$$

Analogous calculations give us the required results for type II. Further, by applying induction, we get

$$\begin{aligned}
&\left(-D^{\mathrm{I}_d} + \frac{d^2}{4}\right)^{\ell}\left(P_m^{(0,l_n+\frac{d}{2}-1)}\left(\frac{2r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}\right)\\
&\qquad\qquad = \left(l_n + 2m + \frac{d}{2}\right)^{2\ell}\left(P_m^{(0,l_n+\frac{d}{2}-1)}\left(\frac{2r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}\right)
\end{aligned}$$

and

$$\left(-D^{\mathrm{II}_d} + \frac{d^2}{4}\right)^{\ell}\left(P_m^{(0,d-1)}\left(\frac{2r}{R}-1\right)\right) = \left(m + \frac{d}{2}\right)^{2\ell}\left(P_m^{(0,d-1)}\left(\frac{2r}{R}-1\right)\right).$$

■

Definition 6.4.4 *For $q \in \mathbb{R}_0^+$, we define the operators*

$$\mathbb{D}^q_{\mathrm{X}_d} := \left(-D^{\mathrm{X}_d} + \frac{d^2}{4}\right)^q,$$

by their eigenvalues

$$\left(\left(-D^{\mathrm{I}_d} + \frac{d^2}{4}\right)^q\right)^{\wedge}(m,n) := \left(l_n + 2m + \frac{d}{2}\right)^{2q}, \quad \mathrm{X} = \mathrm{I},\ \beta = l_n + \frac{d}{2} - 1 \tag{6.31}$$

$$\left(\left(-D^{\mathrm{II}_d} + \frac{d^2}{4}\right)^q\right)^{\wedge}(m,n) := \left(m + \frac{d}{2}\right)^{2q}, \qquad \mathrm{X} = \mathrm{II},\ \beta = d - 1, \tag{6.32}$$

corresponding to the eigenfunctions

$$P_m^{(0,l_n+\frac{d}{2}-1)}\left(\frac{2r^2}{R^2}-1\right)\left(\frac{r}{R}\right)^{l_n}$$

and

$$P_m^{(0,d-1)}\left(\frac{2r}{R}-1\right),$$

respectively.

Next, we define a class of invertible differential operators for the functions on $\mathcal{B}_R^d$, analogously to the operators in the 3-dimensional case defined in Theorem 2.1.3 (see Section 2.1). These operators are the composition of two differential operators, one acting on the angular part and the other on the radial part of the function.

Definition 6.4.5 *We define the operators*

$$\mathbb{A}_{\mathrm{X},d}^{p,q} := \mathbb{B}_d^p \circ \mathbb{D}_{\mathrm{X}_d}^q, \quad p,q \in \mathbb{R}_0^+, \tag{6.33}$$

for the orthonormal systems (6.21) *and* (6.22) *corresponding to the eigenvalues*

$$\left(\mathbb{A}_{\mathrm{I},d}^{p,q}\right)^\wedge(m,n) = \begin{cases} \left(l_0+2m+\frac{d}{2}\right)^{2q}, & n=0, \\ & m\in\mathbb{N}_0, \\ \left(l_n+2m+\frac{d}{2}\right)^{2q}\left((2n+d-2)n(n+d-2)\right)^p, & n\in\mathbb{N}, \\ & m\in\mathbb{N}_0, \end{cases} \tag{6.34}$$

and

$$\left(\mathbb{A}_{\mathrm{II},d}^{p,q}\right)^\wedge(m,n) = \begin{cases} \left(m+\frac{d}{2}\right)^{2q}, & n=0, m\in\mathbb{N}_0, \\ \left(m+\frac{d}{2}\right)^{2q}\left((2n+d-2)n(n+d-2)\right)^p, & n\in\mathbb{N}, m\in\mathbb{N}_0. \end{cases} \tag{6.35}$$

where $\mathbb{B}_d^p$, *defined by the eigenvalues*

$$\mathbb{B}_d^{p\wedge}(n) = \begin{cases} 1, & n=0, \\ \left((2n+d-2)n(n+d-2)\right)^p, & n\in\mathbb{N}, \end{cases} \tag{6.36}$$

is the generalization of the operator defined by (2.3) *and* $\mathbb{D}_{\mathrm{X}_d}^q$ *are given by Definition 6.4.4.*

6.5 Sobolev Space on $\mathcal{B}_R^d$

A Sobolev space on $\mathcal{B}_R^d$, depending on a real sequence $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ and a system of functions $\{G_{m,n,j}^{\mathrm{X},d}\}_{m,n\in\mathbb{N}_0;j=1,\ldots,\mathcal{Z}(d,n)}$, can be defined in the same manner as defined in Definition 1.4.5.

Definition 6.5.1 *A Sobolev space $\mathcal{H}(\{A_{m,n}\}, \mathrm{X}, \mathcal{B}_R^d)$ on $\mathcal{B}_R^d$ is a space of all functions $F \in \mathrm{L}^2(\mathcal{B}_R^d)$ satisfying for all (m, n, j)*

$$\left\langle F, G_{m,n,j}^{\mathrm{X},d} \right\rangle_{\mathrm{L}^2(\mathcal{B}_R^d)} = 0$$

with $A_{m,n} = 0$ or $l_n < 0$ and

$$\sum_{m,n=0}^{\infty} \sum_{j=1}^{\mathcal{Z}(d,n)} A_{m,n}^2 \left\langle F, G_{m,n,j}^{\mathrm{X},d} \right\rangle_{\mathrm{L}^2(\mathcal{B}_R^d)}^2 < +\infty.$$

We denote this space by $\mathcal{H}^d := \mathcal{H}(\{A_{m,n}\}, \mathrm{X}, \mathcal{B}_R^d)$. We now define the summability conditions in higher dimensions, in analogy to Definition 1.4.6, corresponding to the orthonormal basis of type I and II.

Definition 6.5.2 *A real sequence $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ is said to fulfil the summability condition of type* I *if*

$$\sum_{\substack{m,n=0;\, l_n>1-\frac{d}{2} \\ A_{m,n}\neq 0}}^{\infty} A_{m,n}^{-2}(4m + 2l_n + d)(2n + d - 2)^{d-2} \frac{(m + l_n + \frac{d}{2} - 1)^{2m}}{(m!\,)^2} < +\infty \tag{6.37}$$

and of type II *if*

$$\sum_{\substack{m,n=0 \\ A_{m,n}\neq 0}}^{\infty} A_{m,n}^{-2}(2m + d)^{2d-1}(2n + d - 2)^{d-2} < +\infty. \tag{6.38}$$

The summability condition helps us to prove an important result concerning the functions from the Sobolev space $\mathcal{H}^d$.

Lemma 6.5.3 (Sobolev Lemma for d Dimensions). *For a summable sequence $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ and a function $F \in \mathcal{H}^d$, the Fourier series*

$$F(x) = \sum_{m,n=0}^{\infty} \sum_{j=1}^{\mathcal{Z}(d,n)} \left\langle F, G_{m,n,j}^{\mathrm{X},d} \right\rangle_{\mathrm{L}^2(\mathcal{B}_R^d)} G_{m,n,j}^{\mathrm{X},d}(x), \quad x \in \mathcal{B}_R^d \setminus \{0\},$$

is continuous and uniformly convergent on $\mathcal{B}_R^d \setminus \{0\}$.

Proof: For $F \in \mathcal{H}^d$, using the Cauchy-Schwarz inequality (1.17), we get

$$\left| \sum_{m+n \geq M} \sum_{j=1}^{\mathcal{Z}(d,n)} \left\langle F, G^{\mathrm{X},d}_{m,n,j} \right\rangle_{\mathrm{L}^2(\mathcal{B}^d_R)} G^{\mathrm{X},d}_{m,n,j}(x) \right|$$

$$\leq \left(\sum_{m+n \geq M} \sum_{j=1}^{\mathcal{Z}(d,n)} A^2_{m,n} \left\langle F, G^{\mathrm{X},d}_{m,n,j} \right\rangle^2_{\mathrm{L}^2(\mathcal{B}^d_R)} \right)^{\frac{1}{2}} \left(\sum_{\substack{m+n \geq M \\ A_{m,n} \neq 0}} \sum_{j=1}^{\mathcal{Z}(d,n)} A^{-2}_{m,n} \left(G^{\mathrm{X},d}_{m,n,j}(x) \right)^2 \right)^{\frac{1}{2}}$$

$$\leq \|F\|_{\mathcal{H}^d(\mathcal{B}^d_R)} \left(\sum_{\substack{m+n \geq M \\ A_{m,n} \neq 0}} \sum_{j=1}^{\mathcal{Z}(d,n)} A^{-2}_{m,n} \left(G^{\mathrm{X},d}_{m,n,j}(x) \right)^2 \right)^{\frac{1}{2}}.$$

Since the norm of F in the Sobolev space $\mathcal{H}^d$ is finite, we are left with the second term in the above inequality. For a sequence $\{A_{m,n}\}_{m,n \in \mathbb{N}_0}$, we consider the following summation:

$$\sum_{\substack{m+n \geq M \\ A_{m,n} \neq 0}} \sum_{j=1}^{\mathcal{Z}(d,n)} A^{-2}_{m,n} \left(G^{\mathrm{X},d}_{m,n,j}(x) \right)^2 = \sum_{\substack{m+n \geq M \\ A_{m,n} \neq 0}} \sum_{j=1}^{\mathcal{Z}(d,n)} A^{-2}_{m,n} \left(F^{\mathrm{X},d}_{m,n}(|x|) Y^d_{n,j}\left(\frac{x}{|x|} \right) \right)^2.$$

Using (6.16), we have

$$\sum_{\substack{m+n \geq M \\ A_{m,n} \neq 0}} \sum_{j=1}^{\mathcal{Z}(d,n)} A^{-2}_{m,n} \left(G^{\mathrm{X},d}_{m,n,j}(x) \right)^2 = \sum_{\substack{m+n \geq M \\ A_{m,n} \neq 0}} A^{-2}_{m,n} \left(F^{\mathrm{X},d}_{m,n}(|x|) \right)^2 \frac{\mathcal{Z}(d,n)}{\omega_d} P^d_n(\xi \cdot \xi),$$

where $\xi := \frac{x}{|x|}$. Using the fact

$$P^d_n(\xi \cdot \xi) = P^d_n(1) = 1$$

and applying Theorem 1.2.10 for Jacobi polynomials, we arrive at the following inequality:

$$\sum_{\substack{m+n \geq M \\ A_{m,n} \neq 0}} \sum_{j=1}^{\mathcal{Z}(d,n)} A^{-2}_{m,n} \left(G^{\mathrm{X},d}_{m,n,j}(x) \right)^2$$

$$\leq \begin{cases} \sum\limits_{\substack{m+n \geq M \\ A_{m,n} \neq 0}} A^{-2}_{m,n} \frac{4m+2l_n+d}{R^d} \binom{m+l_n+\frac{d}{2}-1}{m}^2 \frac{\mathcal{Z}(d,n)}{\omega_d}, & \mathrm{X} = \mathrm{I}, \\ \sum\limits_{\substack{m+n \geq M \\ A_{m,n} \neq 0}} A^{-2}_{m,n} \frac{2m+d}{R^d} \binom{m+d-1}{m}^2 \frac{\mathcal{Z}(d,n)}{\omega_d}, & \mathrm{X} = \mathrm{II}. \end{cases} \tag{6.39}$$

Now, we can further simplify the terms in the above inequality as follows: for X = I, we have

$$\begin{aligned}
\binom{m+l_n+\frac{d}{2}-1}{m} &= \frac{\Gamma(l_n+\frac{d}{2})}{m!\,\Gamma(l_n+\frac{d}{2})}\cdot\prod_{k=\frac{d}{2}}^{m+\frac{d}{2}-1}(l_n+k)\\
&\leq \frac{(m+l_n+\frac{d}{2}-1)\dots(m+l_n+\frac{d}{2}-1)(m+l_n+\frac{d}{2}-1)}{m!}\\
&= \frac{(m+l_n+\frac{d}{2}-1)^m}{m!}
\end{aligned}$$

and for X = II,

$$\begin{aligned}
\binom{m+d-1}{m} &= \frac{(m+d-1)\dots(m+2)(m+1)}{(d-1)!}\\
&\leq \frac{(2m+d)\dots(2m+d)(2m+d)}{(d-1)!}\\
&= \frac{(2m+d)^{d-1}}{(d-1)!}.
\end{aligned}$$

Simplifying the term $\mathcal{Z}(d,n)$ given by equation (6.8), we get

$$\begin{aligned}
\mathcal{Z}(d,n) &= \frac{(2n+d-2)(n+d-3)!}{n!\,(d-2)!}\\
&= \frac{(2n+d-2)}{(d-2)!}\prod_{k=1}^{d-3}(n+k)\\
&\leq \frac{(2n+d-2)(2n+d-2)^{d-3}}{(d-2)!}\\
&= \frac{(2n+d-2)^{d-2}}{(d-2)!}.
\end{aligned}$$

Using these simplifications, equation (6.39) takes the following form:

$$\begin{aligned}
&\sum_{\substack{m+n\geq M\\ A_{m,n}\neq 0}}\sum_{j=1}^{\mathcal{Z}(d,n)} A_{m,n}^{-2}\left(G_{m,n,j}^{\mathrm{X},d}(x)\right)^2\\
&\quad\leq \begin{cases}\sum\limits_{\substack{m+n\geq M\\ A_{m,n}\neq 0}} A_{m,n}^{-2}\frac{4m+2l_n+d}{R^d}\frac{(m+l_n+\frac{d}{2}-1)^{2m}}{(m!)^2}\frac{(2n+d-2)^{d-2}}{(d-2)!\omega_d}, & \mathrm{X}=\mathrm{I},\\ \sum\limits_{\substack{m+n\geq M\\ A_{m,n}\neq 0}} A_{m,n}^{-2}\frac{2m+d}{R^d}\frac{(2m+d)^{2(d-1)}}{((d-1)!)^2}\frac{(2n+d-2)^{d-2}}{(d-2)!\omega_d}, & \mathrm{X}=\mathrm{II}.\end{cases}
\end{aligned}\tag{6.40}$$

Since $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ satisfies the summability conditions I and II, the term

$$\sum_{\substack{m+n\geq M\\ A_{m,n}\neq 0}} \sum_{j=1}^{\mathcal{Z}(d,n)} A_{m,n}^{-2} \left(G_{m,n,j}^{\mathrm{X},d}(x)\right)^2$$

is convergent for $M, N \to \infty$. This gives us the required result. ■

The Sobolev lemma for d dimensions allows us to state that for every arbitrary but fixed $x \in \mathcal{B}_R^d$, the evaluation functional $\mathcal{L}_x : \mathcal{H}^d \to \mathbb{R}$ is bounded and, consequently, continuous. This statement together with Aronszajn's theorem 1.1.16 infers that the Sobolev space $\mathcal{H}^d$ is a reproducing kernel Hilbert space. Further, Sobolev lemma 6.5.3 and Definition 6.5.1 show that

$$\sum_{\substack{m,n=0\\ A_{m,n}\neq 0}}^{\infty} \sum_{j=1}^{\mathcal{Z}(d,n)} \left(\frac{G_{m,n,j}^{\mathrm{X},d}(x)}{A_{m,n}}\right)^2 < +\infty \tag{6.41}$$

and $\{A_{m,n}^{-1}G_{m,n,j}^{\mathrm{X},d}\}_{m,n\in\mathbb{N}_0, A_{m,n}\neq 0; j=1,2,\ldots,2n+1}$ is a complete system in $\mathcal{H}^d$. Hence, from Theorem 1.1.17, we get the following formula for the reproducing kernel $\mathcal{K}_{\mathcal{H}^d}$:

$$\mathcal{K}_{\mathcal{H}^d}(x,y) = \sum_{\substack{m,n=0,\, l_n\geq 0\\ A_{m,n}\neq 0}}^{\infty} \sum_{j=1}^{\mathcal{Z}(d,n)} \frac{G_{m,n,j}^{\mathrm{X},d}(x) G_{m,n,j}^{\mathrm{X},d}(y)}{A_{m,n}^2}. \tag{6.42}$$

In connection with Definition 2.1.4, we now give the following definition of a Sobolev space on $\mathcal{B}_R^d$ depending on particular sequences:

Definition 6.5.4 *For $p = s$ and $q = \frac{t}{2}$ with $s, t \in \mathbb{R}_0^+$, we define a Sobolev space on $\mathcal{B}_R^d$ depending on the sequences* (6.34) *and* (6.35) *as follows*

$$\mathcal{H}_{s,t}^{X,d}(\mathcal{B}_R^d) := \mathcal{H}\left(\left\{\left(\mathbb{A}_{\mathrm{X},d}^{s,\frac{t}{2}}\right)^{\wedge}(m,n)\right\}, \mathrm{X}, \mathcal{B}_R^d\right). \tag{6.43}$$

We denote the corresponding reproducing kernel of the Sobolev space $\mathcal{H}_{s,t}^{X,d}(\mathcal{B}_R^d)$ by $\mathcal{K} := \mathcal{K}_{\mathcal{H}_{s,t}^{X,d}}$. Based on the Sobolev space (6.43), we now give the definition of the pseudodifferential operators in d dimensions.

Definition 6.5.5 *The operator $\mathcal{A} : \mathcal{H}_{s,t}^{X,d}(\mathcal{B}_R^d) \to \mathcal{H}_{s-\frac{p}{3},t-q}^{X,d}(\mathcal{B}_R^d)$ for $s, t \in \mathbb{R}^+$ and $s \geq \frac{p}{3}$, $t \geq q$, defined by*

$$\mathcal{A}F = \sum_{m,n=0}^{\infty} \sum_{j=1}^{\mathcal{Z}(d,n)} A_{m,n} \left\langle F, G_{m,n,j}^{\mathrm{X},d}\right\rangle_{\mathrm{L}^2(\mathcal{B}_R^d)} G_{m,n,j}^{\mathrm{X},d}$$

is said to be a pseudodifferential operator of type (X, d) *with respect to the orthonormal basis system of type* (X, d)*, if for all* $m, n \in \mathbb{N}_0$ *its eigenvalues satisfy*

$$c_1(n + c_2)^p(l_n + m + c_3)^q \leq |A_{m,n}| \leq c_4(n + c_5)^p(l_n + m + c_6)^q, \quad \mathrm{X} = \mathrm{I},$$

where $\left\langle F, G^{\mathrm{X},d}_{m,n,j} \right\rangle_{\mathrm{L}^2(\mathcal{B}^d_R)} = 0$ *for all* $l_n < 0$ *(see Definition 6.5.1) and*

$$c_1(n + c_2)^p(m + c_3)^q \leq |A_{m,n}| \leq c_4(n + c_5)^p(m + c_6)^q, \quad \mathrm{X} = \mathrm{II}.$$

Here, all c_i *are constants and* $p, q \in \mathbb{R}^+$ *are called the angular and radial orders of the operator, respectively.*

While generalizing the idea of Sobolev space and pseudodifferential operators to d dimensions, we realized that working in higher dimensions does not effect the properties (be it isometry or the radial and angular orders of the differential operators (see Theorem 2.1.10)) of the operators. Hence, all the properties from Section 2.1 can be extended for the operators defined by Definition 6.4.5 to any dimension d.

6.6 Discrepancy in Higher Dimensions

The concept of discrepancy (generalized and weighted) and the related result in d dimension is an easy extension of the results in Sections 2.2 and 2.3. Suppose we have a function F on the ball $\mathcal{B}^d_R$. Then, its integral value can be approximated as

$$\int_{\mathcal{B}^d_R} F(x)\mathrm{d}x \approx \sigma_d \sum_{k=1}^{N} \alpha_k F(x_k), \tag{6.44}$$

where σ_d denotes the volume of $\mathcal{B}^d_R$ and α_k are the weights with $\sum_{k=1}^N \alpha_k = 1$. The following theorem gives an estimate of the quadrature error for (6.44). This result is analogous to Theorem 2.3.1, limited to the case $d = 3$.

Theorem 6.6.1 *Let* $\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)$ *be a Sobolev space defined by Definition 6.5.4 with* $s \geq \frac{p}{3}$ *,* $t \geq q$ *and a summable sequence* $\{(\mathbb{A}^{s,\frac{t}{2}}_{\mathrm{X},d})^\wedge(m, n)\}_{m,n\in\mathbb{N}_0}$*. Further, let* $\mathcal{A}$ *be a pseudodifferential operator (see Definition 6.5.5) on* $\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)$ *with summable eigenvalues* $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$*, which are zero if and only if the sequence* $\{(\mathbb{A}^{s,\frac{t}{2}}_{\mathrm{X},d})^\wedge(m, n)\}_{m,n\in\mathbb{N}_0}$ *is zero and* $A_{0,0} \neq 0$*. Then, for any function*

$F \in \mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)$, we have

$$\left| \frac{1}{\sigma_d} \int_{\mathcal{B}^d_R} F(x)\mathrm{d}x - \sum_{k=1}^{N} \alpha_k F(x_k) \right| \leq \|\mathcal{A}F\|_{\mathrm{L}^2(\mathcal{B}^d_R)} \left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n \geq 0}} \frac{1}{A^2_{m,n}} \sum_{j=1}^{\mathcal{Z}(d,n)} \sum_{i,k=1}^{N} \alpha_i \alpha_k G^{\mathrm{X},d}_{m,n,j}(x_i) G^{\mathrm{X},d}_{m,n,j}(x_k) \right)^{\frac{1}{2}}. \tag{6.45}$$

Proof: The result can be proved on similar lines as in Theorem 2.2.1. ■

Now, similar to the idea defined in Definition 2.2.2, we give the following definition of a discrepancy in d dimensions.

Definition 6.6.2 *Let $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ be a real summable sequence such that $A_{m,n} \neq 0$ represents the eigenvalues for a pseudodifferential operator $\mathcal{A}$, then the discrepancy of a set of N points $\mathcal{P}_N = \{x_1, x_2, \ldots, x_N\} \subset \mathcal{B}^d_R$ together with weights $\{\alpha_1, \alpha_2, \ldots, \alpha_N\} \subset \mathbb{R}$, is defined as*

$$D_w(\mathcal{P}_N, \mathrm{X}, \mathcal{A}) := \left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n \geq 0}} \frac{1}{A^2_{m,n}} \sum_{j=1}^{\mathcal{Z}(d,n)} \sum_{i,k=1}^{N} \alpha_i \alpha_k G^{\mathrm{X},d}_{m,n,j}(x_i) G^{\mathrm{X},d}_{m,n,j}(x_k) \right)^{\frac{1}{2}}. \tag{6.46}$$

Remark 6.6.3 *1. For the weights $\alpha_i = \alpha_k = \frac{1}{N}$, the discrepancy in* (6.46) *takes the following form:*

$$D(\mathcal{P}_N, \mathrm{X}, \mathcal{A}) := \left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n \geq 0}} \frac{1}{A^2_{m,n}} \sum_{j=1}^{\mathcal{Z}(d,n)} \sum_{i,k=1}^{N} \frac{G^{\mathrm{X},d}_{m,n,j}(x_i) G^{\mathrm{X},d}_{m,n,j}(x_k)}{N^2} \right)^{\frac{1}{2}}. \tag{6.47}$$

2. If we apply the addition theorem (6.16)*, equation* (6.47) *yields*

$$D(\mathcal{P}_N, \mathrm{X}, \mathcal{A}) = \left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n \geq 0}} \sum_{i,k=1}^{N} \frac{F^{\mathrm{X},d}_{m,n}(|x_i|) F^{\mathrm{X},d}_{m,n}(|x_k|)}{A^2_{m,n} N^2} \frac{\mathcal{Z}(d,n)}{\omega_d} P^d_n (\xi_i \cdot \xi_k) \right)^{\frac{1}{2}}, \tag{6.48}$$

with $\xi_i = \frac{x_i}{|x_i|}$.

These formulae for discrepancies with constant or variable weights enable us to take our theory of equidistribution to any dimension $d \geq 3$. In order to have some numerical tests, we take the simple lattice (equation (3.1)). It is easy to generalize the simple lattice to higher dimensions, which is actually the justification for taking this particular grid for the numerical tests. For dimension $d \geq 3$, the simple lattice is given by

$$\theta_{i,d-2} := \frac{i\pi}{P}, \quad 0 \leq i \leq P,$$
$$\phi_j := \frac{2j\pi}{P}, \quad 0 \leq j \leq P.$$

We distribute the points on the unit ball $\mathcal{B}^4$ by replacing the value P with $\lfloor rP \rfloor$, where $r \in [0,1]$ (for details see Section 3.1) and we calculate the discrepancies for the resulting grid using equation (6.47). For the orthonormal system I with the particular value $l_n = n$ in dimension $d = 4$, (6.48) takes the form

$$D(\mathcal{P}_N, \mathrm{I}, \mathcal{A}) = \frac{1}{\pi N}\left[\sum_{i,k=1}^{N}\left(\sum_{m,n=0}^{\infty}\frac{(n+2m+2)(n+1)^2}{A_{m,n}^2}(|x_i||x_k|)^n \right.\right.$$
$$\left.\left. \times P_m^{(0,n+1)}(2|x_i|^2-1)P_m^{(0,n+1)}(2|x_k|^2-1)P_n^4\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right) - \frac{2}{A_{0,0}^2}\right)\right]^{\frac{1}{2}} \quad (6.49)$$

and for type II,

$$D(\mathcal{P}_N, \mathrm{II}, \mathcal{A}) = \frac{1}{\pi N}\left[\sum_{i,k=1}^{N}\left(\sum_{m,n=0}^{\infty}\frac{(m+2)(n+1)^2}{A_{m,n}^2}P_m^{(0,3)}(2|x_i|-1)\right.\right.$$
$$\left.\left. \times P_m^{(0,3)}(2|x_k|-1)P_n^4\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right) - \frac{2}{A_{0,0}^2}\right)\right]^{\frac{1}{2}}. \quad (6.50)$$

For the numerical tests, we have to truncate (as in Chapter 2) the infinite series in the above mentioned discrepancy formulae up to certain degrees $\mathcal{M}$ and $\mathcal{N}$ of Jacobi and Legendre polynomials, respectively. In our calculations, we take $\mathcal{M} = 10$ and $\mathcal{N} = 10$ for both the types I and II. Also, we have to choose a particular pseudodifferential operator. Here, we use the pseudodifferential operator $\mathcal{A} = \mathbb{A}_{\mathrm{X},4}^{p,q}$ (see Definition 6.4.5) with $p = 1$ and $q = 1$ and the corresponding eigenvalues. The values of p and q are chosen in such a way, that the series in (6.49) and (6.50) are convergent in m and n. Substituting

$$A_{m,n} := \left(\mathbb{A}_{\mathrm{I},4}^{1,1}\right)^{\wedge}(m,n)$$

in equation (6.49), we get

$$D(\mathcal{P}_N, \mathrm{I}, \mathcal{A}) = \frac{1}{2\pi N}\left[\sum_{i,k=1}^{N}\left(\sum_{m=0}^{\mathcal{M}}\frac{1}{(m+1)^3}P_m^{(0,1)}(2|x_i|^2-1)P_m^{(0,1)}(2|x_k|^2-1)\right.\right.$$
$$+\sum_{m=0}^{\mathcal{M}}\sum_{n=1}^{\mathcal{N}}\frac{2}{(n+2m+2)^3n^2(n+2)^2}\left(|x_i||x_k|\right)^n P_m^{(0,n+1)}(2|x_i|^2-1)$$
$$\left.\left.\times P_m^{(0,n+1)}(2|x_k|^2-1)P_n^4\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)-1\right)\right]^{\frac{1}{2}}, \quad (6.51)$$

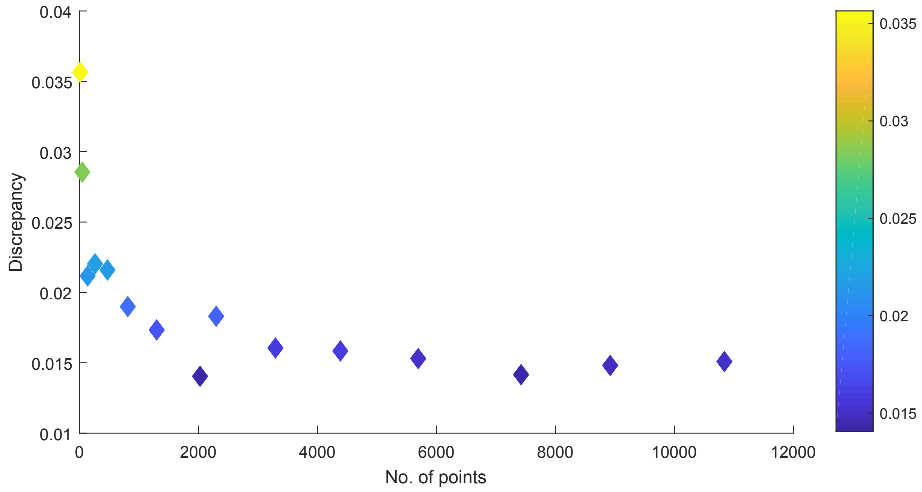
and for

$$A_{m,n} := \left(\mathbb{A}_{\mathrm{II},4}^{1,1}\right)^{\wedge}(m,n)$$

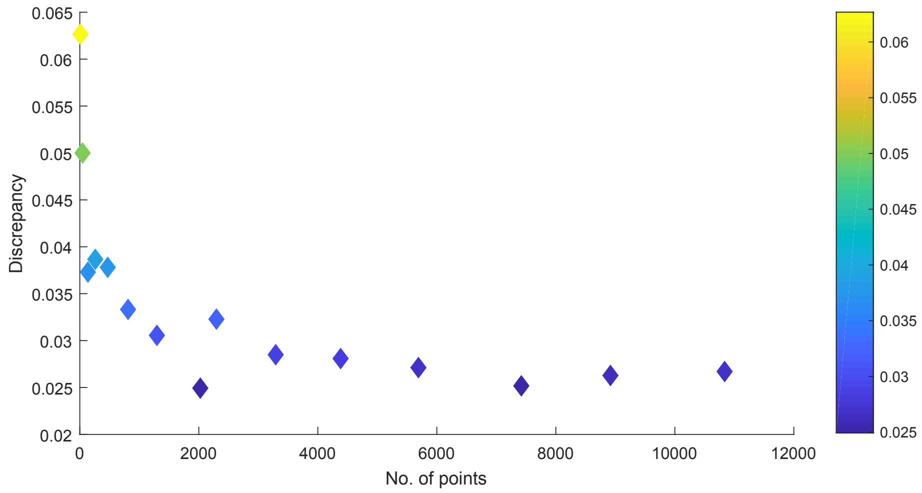
equation (6.50) yields

$$D(\mathcal{P}_N, \mathrm{II}, \mathcal{A}) = \frac{1}{\pi N}\left[\sum_{i,k=1}^{N}\left(\left(\sum_{m=0}^{\mathcal{M}}\frac{1}{(m+2)^3}P_m^{(0,3)}(2|x_i|-1)P_m^{(0,3)}(2|x_k|-1)\right)\right.\right.$$
$$\left.\left.\times\left(1+\sum_{n=1}^{\mathcal{N}}\frac{1}{2n^2(n+2)^2}P_n^4\left(\frac{x_i}{|x_i|}\cdot\frac{x_k}{|x_k|}\right)\right)-\frac{1}{4}\right)\right]^{\frac{1}{2}}. \quad (6.52)$$

Figure 6.1 shows the calculated discrepancies for an increasing number of grid points on a 4-dimensional unit ball.



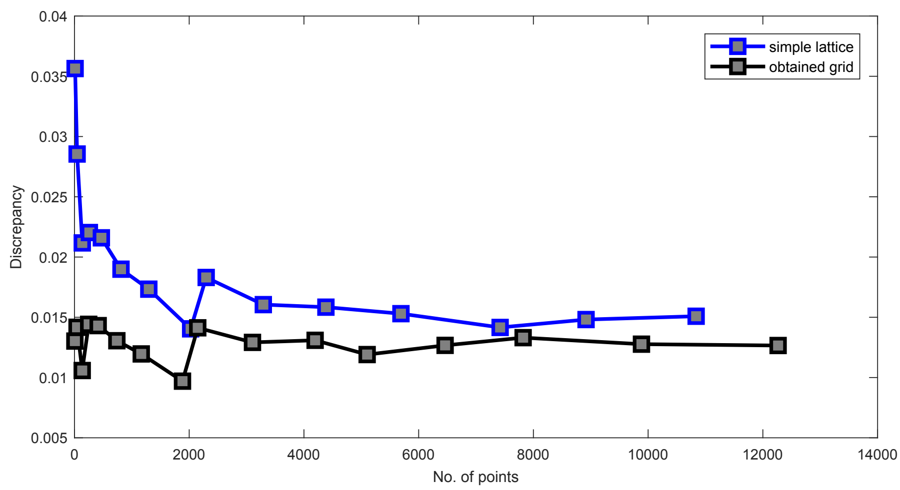
(a)



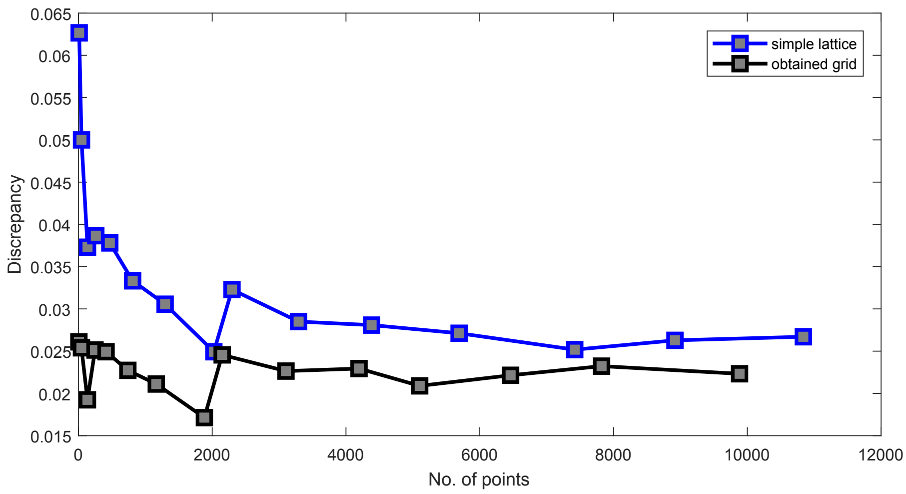
(b)

Figure 6.1: The behaviour of the generalized discrepancies for the simple lattice in dimension $d = 4$ corresponding to the orthonormal basis system of type I represented in (a) and for the orthonormal basis system of type II shown in (b). The colourbar represents the values of the discrepancies.

We have already discussed different algorithms in Chapter 3 that work for minimizing the discrepancies of the grids on the ball. We choose here Algorithm 1 (see Section 4.1) for numerical computation as it gives better results in comparison to other methods. We then compared the discrepancies of the resulting grids with the modified simple lattice. Figure 6.2 shows the comparisons of the discrepancies calculated for types I and II.



(a)



(b)

Figure 6.2: The plots show the comparison between the discrepancy estimates of the simple lattice and the grid obtained from Algorithm 1 for dimension $d = 4$. The results corresponding to the orthonormal basis system of type I are shown in (a) and for the orthonormal basis system of type II in (b).

Furthermore, we tested the BFGS method for the 4-dimensional case. Using this method, we minimize our objective function $f_{\text{obj,X}} := D^2\left(\mathcal{P}_N, \mathbb{A}^{1,1}_{\text{X},4}\right)$ with the help of its gradient. For the computation of the gradient, we proceed as follows: as our objective function comprised of Jacobi and Legendre polynomials, which can be written in terms of Gegenbauer polynomials (see (6.5)), we use equations (1.35) and (1.38) to find their gradients. The gradients for Jacobi polynomials of type I and II, respectively are

$$\begin{aligned}\nabla_{x_t} P_m^{(0,n+1)}(2|x_i|^2-1) &= \frac{\Gamma(n+m+3)}{2\,\Gamma(n+m+2)}\, P_{m-1}^{(1,n+2)}(2|x_i|^2-1)\, 4\, x_i^{\mathrm{T}}\, \nabla_{x_t} x_i \\ &= 2(n+m+2) P_{m-1}^{(1,n+2)}(2|x_i|^2-1)\, x_i^{\mathrm{T}}\, \nabla_{x_t} x_i, \qquad (6.53)\end{aligned}$$

where $\nabla_{x_t} x_i = \delta_{ti}\, I$ and $t = 1, 2, \ldots, N$ and

$$\begin{aligned}\nabla_{x_t} P_m^{(0,3)}(2|x_i|-1) &= \frac{\Gamma(m+5)}{2\,\Gamma(m+4)}\, P_{m-1}^{(1,4)}(2|x_i|-1)\, 2 \left(\frac{x_i}{|x_i|}\right)^{\mathrm{T}} \nabla_{x_t} x_i \\ &= (m+4) P_{m-1}^{(1,4)}(2|x_i|-1) \left(\frac{x_i}{|x_i|}\right)^{\mathrm{T}} \nabla_{x_t} x_i. \qquad (6.54)\end{aligned}$$

From (6.5), we can write

$$P_n^4\left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right) = \frac{1}{n+1} C_n^1 \left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right).$$

Further, we use Theorem 1.1.2 and the formula for the surface gradient of a zonal function

$$\nabla_\xi^* F(\xi \cdot \eta) = F'(\xi \cdot \eta)[\eta - (\xi \cdot \eta)\xi] \qquad (6.55)$$

from [47] and get the gradient of the Gegenbauer polynomials as

$$\begin{aligned}\nabla_{x_t} C_n^1\left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right) &= \frac{2}{|x_t|} C_{n-1}^2 \left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right) \nabla^*_{\frac{x_t}{|x_t|}} \left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right) \\ &= \frac{2}{|x_t|} C_{n-1}^2 \left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right) \left[\delta_{it} \left(\frac{x_k}{|x_k|} - \left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right) \frac{x_i}{|x_i|}\right)\right. \\ &\quad \left. + \delta_{kt} \left(\frac{x_i}{|x_i|} - \left(\frac{x_i}{|x_i|} \cdot \frac{x_k}{|x_k|}\right) \frac{x_k}{|x_k|}\right)\right]. \qquad (6.56)\end{aligned}$$

Moreover, we use equation (4.11) for the gradient of term $(|x_i||x_k|)^n$ in the objective function $f_{\mathrm{obj,I}}$. In combination with the above calculations, the gradient of $f_{\text{obj,I}}$ is given by

$$\frac{1}{4\pi^2N^2}\sum_{i=1}^{N}\Bigg[\sum_{m=1}^{\mathcal{M}}\frac{4(m+2)}{(m+1)^3}P_m^{(0,1)}(2|x_i|^2-1)P_{m-1}^{(1,2)}(2|x_t|^2-1)x_t$$
$$+\sum_{m=0}^{\mathcal{M}}\sum_{n=1}^{\mathcal{N}}\frac{4n}{(n+2m+2)^3n^2(n+2)^2}\frac{(|x_i||x_t|)^{n-1}}{n+1}|x_i|\frac{x_t}{|x_t|}P_m^{(0,n+1)}(2|x_i|^2-1)$$
$$\times P_m^{(0,n+1)}(2|x_t|^2-1)C_n^1\left(\frac{x_i}{|x_i|}\cdot\frac{x_t}{|x_t|}\right)+\sum_{m=1}^{\mathcal{M}}\sum_{n=1}^{\mathcal{N}}\frac{8(n+m+2)}{(n+2m+2)^3n^2(n+2)^2}$$
$$\times\frac{(|x_i||x_t|)^n}{n+1}P_m^{(0,n+1)}(2|x_i|^2-1)P_{m-1}^{(1,n+2)}(2|x_t|^2-1)\,x_t\,C_n^1\left(\frac{x_i}{|x_i|}\cdot\frac{x_t}{|x_t|}\right)$$
$$+\sum_{m=0}^{\mathcal{M}}\sum_{n=1}^{\mathcal{N}}\frac{4}{(n+2m+2)^3n^2(n+2)^2}P_m^{(0,n+1)}(2|x_i|^2-1)P_m^{(0,n+1)}(2|x_t|^2-1)$$
$$\times\frac{(|x_i||x_t|)^n}{|x_t|}\left(\frac{x_i}{|x_i|}-\left(\frac{x_i}{|x_i|}\cdot\frac{x_t}{|x_t|}\right)\frac{x_t}{|x_t|}\right)\frac{1}{n+1}C_{n-1}^2\left(\frac{x_i}{|x_i|}\cdot\frac{x_t}{|x_t|}\right)\Bigg]$$

and the gradient of $f_{\text{obj,II}}$ is

$$\frac{2}{\pi^2N^2}\sum_{i=1}^{N}\Bigg[\sum_{m=1}^{\mathcal{M}}\frac{m+4}{(m+2)^3}P_m^{(0,3)}(2|x_i|-1)P_{m-1}^{(1,4)}(2|x_t|-1)\frac{x_t}{|x_t|}$$
$$\left(1+\sum_{n=1}^{\mathcal{N}}\frac{1}{2n^2(n+2)^2(n+1)}C_n^1\left(\frac{x_i}{|x_i|}\cdot\frac{x_t}{|x_t|}\right)\right)$$
$$+\sum_{m=0}^{\mathcal{M}}\sum_{n=1}^{\mathcal{N}}\frac{1}{(m+2)^32n^2(n+2)^2(n+1)}P_m^{(0,3)}(2|x_i|-1)P_m^{(0,3)}(2|x_t|-1)$$
$$\times\left(\frac{x_i}{|x_i|}-\left(\frac{x_i}{|x_i|}\cdot\frac{x_t}{|x_t|}\right)\frac{x_t}{|x_t|}\right)\frac{1}{|x_t|}C_{n-1}^2\left(\frac{x_i}{|x_i|}\cdot\frac{x_t}{|x_t|}\right)\Bigg],$$

for $t = 1, 2, \ldots, N$. We use the BFGS method to minimize the objective functions along with the LDL^{T} method to update the Hessian and Wolfe weak conditions for computing the line search, which is virtually the best combination according to our previous results (for details see Chapter 4). As an example, we have taken here a starting grid of 811 points on a 4-dimensional unit ball. Figures 6.3 and 6.4 show the results for the objective functions $f_{\text{obj,I}}$ and $f_{\text{obj,II}}$.

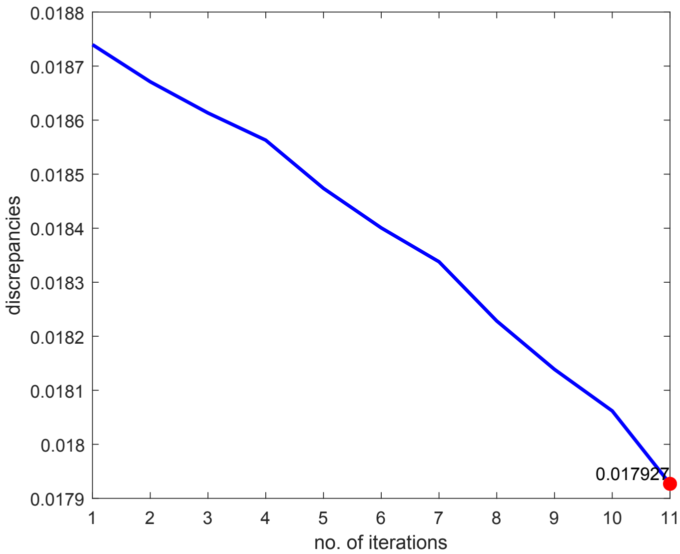


Figure 6.3: The plot shows the behaviour of $f_{\mathrm{obj,I}}$ corresponding to the number of iterations. The red point represents the minimum value of $f_{\mathrm{obj,I}}$ after satisfying the stopping criterion with tolerance level 10^{-11}.

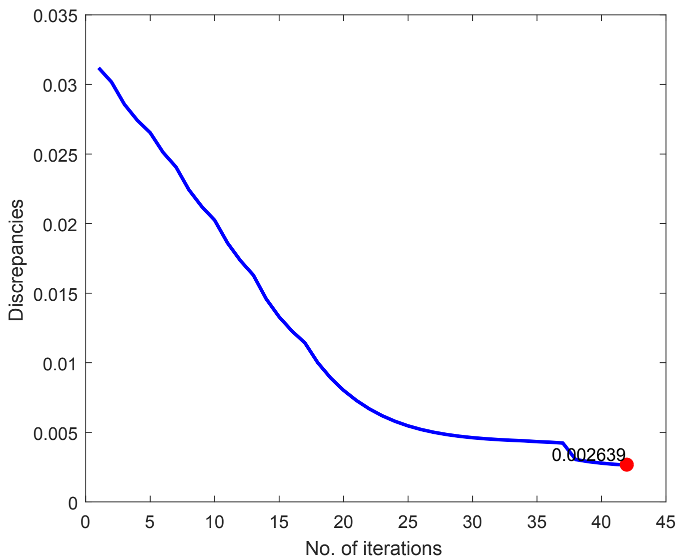


Figure 6.4: The plot shows the behaviour of $f_{\mathrm{obj,II}}$ corresponding to the number of iterations. The red point represents the minimum value of $f_{\mathrm{obj,II}}$ after satisfying the stopping criterion with tolerance level 10^{-5}.

From the above tests, it is evident that these methods show favourable results also in higher dimensions.

6.7 Numerical Properties of the Generalized Discrepancy

As we extend the equidistribution theory and related results to a d-dimensional ball, we also investigate some interesting numerical properties of the generalized discrepancy in d dimensions. The analysis of these properties and the construction of the following results are similar to those used for the spherical case in [12].

6.7.1 Worst-Case Cubature Error

We consider a weighted cubature rule $\mathcal{Q}_{N,d}$ on the ball $\mathcal{B}_R^d$ defined as

$$\mathcal{Q}_{N,d}(F) := \sum_{i=1}^{N} \alpha_i F(x_i), \quad F \in \mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d), \tag{6.57}$$

with weights $\alpha_i \in \mathbb{R}$ such that $\sum_{i=1}^{N} \alpha_i = 1$ and points $x_i \in \mathcal{B}_R^d$. Further, we choose $Q_{N,d}$ as an approximation to the integral of a function $F \in \mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)$ given by

$$\mathcal{I}(F) := \int_{\mathcal{B}_R^d} F(x)\,\mathrm{d}\sigma_d^*(x), \tag{6.58}$$

σ_d^* being the probability measure ($\sigma_d^*(\cdot) = \frac{1}{\sigma_d}\sigma_d(\cdot)$ (see Chapter 5)). Note that this approximation is exact for a constant function F.

Definition 6.7.1 *Let $\mathcal{Q}_{N,d}$ and $\mathcal{I}$ be as defined above, then the worst case error of a function F in the Sobolev space $\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)$ is defined as*

$$\mathcal{E}(\mathcal{Q}_{N,d}) := \sup\left\{ |(\mathcal{I} - \mathcal{Q}_{N,d})F| : F \in \mathcal{H}_{s,t}^{\mathrm{X},d}, \|F\|_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)} \leq 1 \right\}.$$

Definition 6.7.2 *Let $\{x_i\}_{i\geq 1}$ be i.i.d. random points on the ball $\mathcal{B}_R^d$. For each sample of N points $\mathcal{P}_N \subset \{x_i\}_{i\geq 1}$, let $\mathcal{Q}_{N,d}$ be the corresponding weighted quadrature rule as defined by* (6.57) *and $\mathcal{E}$ be the worst case error from Definition 6.7.1. Then we define*

$$\mathcal{E}^{\mathrm{avg}}(\mathcal{Q}_{N,d}) := \left[\mathbb{E}\left(\mathcal{E}(\mathcal{Q}_{N,d})\right)^2\right]^{\frac{1}{2}}. \tag{6.59}$$

Following the results in [12, 47, 66] for the case of a sphere, we derive the corresponding result for the domain of a ball.

Theorem 6.7.3 *Let $\mathcal{P}_N = \{x_1, x_2, \ldots, x_N\}$ be a set of points in $\mathcal{B}_R^d$ and $\mathcal{A}$ be a pseudodifferential operator on $\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)$ satisfying the conditions stated in Theorem 6.6.1, then the worst case error $\mathcal{E}$ for the cubature rule $\mathcal{Q}_{N,d}$ is exactly the discrepancy, i.e.*

$$\mathcal{E}(\mathcal{Q}_{N,d}) = D_w(\mathcal{P}_N, \mathcal{A}). \tag{6.60}$$

For the type $\mathrm{X} = \mathrm{I}$, we require a sufficient condition of $l_0 = 0$.

Proof: Using the equations (6.57) and (6.58), we can write

$$\mathcal{I}(F) - \mathcal{Q}_{N,d}(F) = \int_{\mathcal{B}_R^d} F(x)\,\mathrm{d}\sigma_d^*(x) - \sum_{i=1}^{N} \alpha_i F(x_i).$$

Now, in connection with Theorem 1.1.18, we can write

$$\begin{aligned}
(\mathcal{I} - \mathcal{Q}_{N,d})(F) &= \langle F, (\mathcal{I} - \mathcal{Q}_{N,d})_x\, \mathcal{K}(x, \cdot)\rangle_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)} \\
&= \left\langle F, \int_{\mathcal{B}_R^d} \mathcal{K}(x, \cdot)\,\mathrm{d}\sigma_d^*(x) - \sum_{i=1}^{N} \alpha_i \mathcal{K}(\cdot, x_i) \right\rangle_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)} \\
&= \langle F, \wp\rangle_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)},
\end{aligned}$$

where $\wp := \int_{\mathcal{B}_R^d} \mathcal{K}(x, \cdot)\,\mathrm{d}\sigma_d^*(x) - \sum_{i=1}^{N} \alpha_i \mathcal{K}(\cdot, x_i)$. Hence, by Definition 6.7.1, we get

$$\begin{aligned}
\mathcal{E}(\mathcal{Q}_{N,d}) &= \sup\left\{ \left| \langle F, \wp\rangle_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)} \right| : F \in \mathcal{H}_{s,t}^{\mathrm{X},d}, \|F\|_{\mathcal{H}_{s,t}^{\mathrm{X},d}} \leq 1 \right\} \\
&= \|\wp\|_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)} \\
&= \langle \wp, \wp\rangle^{\frac{1}{2}}_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)} \\
&= \langle (\mathcal{I} - \mathcal{Q}_{N,d})_x\, \mathcal{K}(x, \cdot), (\mathcal{I} - \mathcal{Q}_{N,d})_y\, \mathcal{K}(y, \cdot)\rangle^{\frac{1}{2}}_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)}.
\end{aligned} \tag{6.61}$$

Again using Theorem 1.1.18, for the continuous functional $(\mathcal{I} - \mathcal{Q}_{N,d})$ and the function $(\mathcal{I} - \mathcal{Q}_{N,d})_x\, \mathcal{K}(x, \cdot) \in \mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)$, we obtain

$$\begin{aligned}
&(\mathcal{I} - \mathcal{Q}_{N,d})_y \left[(\mathcal{I} - \mathcal{Q}_{N,d})_x\, \mathcal{K}(x, y)\right] \\
&\qquad = \langle (\mathcal{I} - \mathcal{Q}_{N,d})_x\, \mathcal{K}(x, \cdot), (\mathcal{I} - \mathcal{Q}_{N,d})_y\, \mathcal{K}(y, \cdot)\rangle_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)}.
\end{aligned} \tag{6.62}$$

This results in the following equation:

$$\begin{aligned}\mathcal{E}(\mathcal{Q}_{N,d}) &= \left[(\mathcal{I}-\mathcal{Q}_{N,d})_y(\mathcal{I}-\mathcal{Q}_{N,d})_x\,\mathcal{K}(x,y)\right]^{\frac{1}{2}}\\ &= \Bigg[\int_{\mathcal{B}_R^d}\left(\int_{\mathcal{B}_R^d}\mathcal{K}(x,y)\,\mathrm{d}\sigma_d^*(x)\right)\mathrm{d}\sigma_d^*(y) - 2\sum_{i=1}^{N}\alpha_i\int_{\mathcal{B}_R^d}\mathcal{K}(x,y)\,\mathrm{d}\sigma_d^*(y)\\ &\qquad + \sum_{i=1}^{N}\sum_{k=1}^{N}\alpha_i\alpha_k\mathcal{K}(x_i,x_k)\Bigg]^{\frac{1}{2}}. \end{aligned} \tag{6.63}$$

Next, we require to evaluate the integral of the reproducing kernel $\mathcal{K}$ as the first two terms in the above equation depend on it. Using equation (6.42), we proceed as follows

$$\int_{\mathcal{B}_R^d}\mathcal{K}(x,y)\,\mathrm{d}\sigma_d^*(x) = \int_{\mathcal{B}_R^d}\sum_{\substack{m,n=0\\ l_n\geq 0}}^{\infty}\sum_{j=1}^{\mathcal{Z}(d,n)}\frac{1}{A_{m,n}^2}G_{m,n,j}^{\mathrm{X},d}(x)G_{m,n,j}^{\mathrm{X},d}(y)\,\mathrm{d}\sigma_d^*(x). \tag{6.64}$$

We have here two cases, depending on the two types of orthonormal systems I and II. We consider first the case for X = II. Using equation (6.22) and the fact that $G_{0,0,1}^{\mathrm{II},d} = \sqrt{\frac{d}{\omega_d R^d}}$, we further calculate the integral and obtain

$$\begin{aligned}&\int_{\mathcal{B}_R^d}\mathcal{K}(x,y)\,\mathrm{d}\sigma_d^*(x)\\ &\quad= \sqrt{\frac{\omega_d R^d}{d}}\int_{\mathcal{B}_R^d}\sum_{m,n=0}^{\infty}\sum_{j=1}^{\mathcal{Z}(d,n)}\frac{1}{A_{m,n}^2}G_{m,n,j}^{\mathrm{II},d}(x)G_{0,0,1}^{\mathrm{II},d}(x)G_{m,n,j}^{\mathrm{II},d}(y)\,\mathrm{d}\sigma_d^*(x).\end{aligned}$$

Now the uniform convergence of the series (see Theorem 6.5.3) allows us to interchange the order of summation and the integral.

$$\begin{aligned}&\int_{\mathcal{B}_R^d}K(x,y)\,\mathrm{d}\sigma_d^*(x)\\ &\quad= \sqrt{\frac{\omega_d R^d}{d}}\sum_{m,n=0}^{\infty}\sum_{j=1}^{\mathcal{Z}(d,n)}\frac{1}{A_{m,n}^2}G_{m,n,j}^{\mathrm{II},d}(y)\int_{\mathcal{B}_R^d}G_{m,n,j}^{\mathrm{II},d}(x)G_{0,0,1}^{\mathrm{II},d}(x)\,\mathrm{d}\sigma_d^*(x)\\ &\quad= \sqrt{\frac{\omega_d R^d}{d}}\frac{1}{A_{0,0}^2}G_{0,0,1}^{\mathrm{II},d}(y)\int_{\mathcal{B}_R^d}\left(G_{0,0,1}^{\mathrm{II},d}(x)\right)^2\mathrm{d}\sigma_d^*(x)\\ &\quad= \frac{d}{\omega_d R^d}\frac{1}{A_{0,0}^2}\int_{\mathcal{B}_R^d}\mathrm{d}\sigma_d^*(x)\\ &\quad= \frac{d}{\omega_d R^d}\frac{1}{A_{0,0}^2}.\end{aligned} \tag{6.65}$$

As a result, equation (6.63) yields

$$\begin{aligned}\mathcal{E}(\mathcal{Q}_{N,d}) &= \left[\frac{d}{\omega_d R^d}\frac{1}{A_{0,0}^2} - 2\cdot\frac{d}{\omega_d R^d}\frac{1}{A_{0,0}^2} + \sum_{i=1}^{N}\sum_{k=1}^{N}\alpha_i\alpha_k\mathcal{K}(x_i,x_k)\right]^{\frac{1}{2}}\\ &= \left[-\frac{d}{\omega_d R^d}\frac{1}{A_{0,0}^2} + \sum_{i=1}^{N}\sum_{k=1}^{N}\alpha_i\alpha_k\mathcal{K}(x_i,x_k)\right]^{\frac{1}{2}}\\ &= D_w(\mathcal{P}_N,\mathrm{II},\mathcal{A}).\end{aligned}$$

Similarly, we proceed for the case $\mathrm{X}=\mathrm{I}$. With the help of equation (6.21), the value of $G_{m,n,j}^{\mathrm{I},d}$ at $(m,n,j)=(0,0,1)$ is given by $G_{0,0,1}^{\mathrm{I},d}(x)=\sqrt{\frac{2l_0+d}{\omega_d R^d}}\left(\frac{|x|}{R}\right)^{l_0}$. The condition $l_0=0$ yields $G_{0,0,1}^{\mathrm{I},d}=\sqrt{\frac{d}{\omega_d R^d}}$. Using this value to calculate the integral in (6.64), we obtain

$$\begin{aligned}&\int_{\mathcal{B}_R^d}\mathcal{K}(x,y)\mathrm{d}\sigma_d^*(x)\\ &= \sqrt{\frac{\omega_d R^d}{d}}\int_{\mathcal{B}_R^d}\sum_{\substack{m,n=0\\ l_n\geq 0}}^{\infty}\sum_{j=1}^{\mathcal{Z}(d,n)}\frac{1}{A_{m,n}^2}G_{m,n,j}^{\mathrm{I},d}(x)G_{0,0,1}^{\mathrm{I},d}(x)G_{m,n,j}^{\mathrm{I},d}(y)\,\mathrm{d}\sigma_d^*(x)\\ &= \sqrt{\frac{\omega_d R^d}{d}}\sum_{\substack{m,n=0\\ l_n\geq 0}}^{\infty}\sum_{j=1}^{\mathcal{Z}(d,n)}\frac{1}{A_{m,n}^2}\int_{\mathcal{B}_R^d}G_{m,n,j}^{\mathrm{I},d}(x)G_{0,0,1}^{\mathrm{I},d}(x)\,\mathrm{d}\sigma_d^*(x)G_{m,n,j}^{\mathrm{I},d}(y).\end{aligned}$$

This leads us to the following equation

$$\int_{\mathcal{B}_R^d}\mathcal{K}(x,y)\,\mathrm{d}\sigma_d^*(x) = \frac{d}{\omega_d R^d}\frac{1}{A_{0,0}^2}. \tag{6.66}$$

Consequently, we obtain

$$\mathcal{E}(\mathcal{Q}_{N,d}) = D_w(\mathcal{P}_N,\mathrm{I},\mathcal{A}).$$

This completes the proof. ■

Remark 6.7.4 *If $\alpha_i=\frac{1}{N}$ for all i, then*

$$\mathcal{E}(\mathcal{Q}_{N,d}) = D(\mathcal{P}_N,\mathrm{X},\mathcal{A}).$$

For $N=0$, we formally set $\mathcal{Q}_{0,d}(F)=0$, so the initial error is given as norm of the integral $\mathcal{I}$

$$\mathcal{E}(\mathcal{Q}_{0,d}) = \sup\left\{|\mathcal{I}(F)| : F\in\mathcal{H}_{s,t}^{\mathrm{X},d},\, \|F\|_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)}\leq 1\right\}.$$

Theorem 1.1.18 tells us that $\mathcal{I}(F) = \langle F, \mathcal{I}_x\mathcal{K}(x,\cdot)\rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}}$. Thus, using that $F \in \mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)$ and equations (6.65) and (6.66), we obtain

$$\begin{aligned}\mathcal{E}(\mathcal{Q}_{0,d}) &= \|\mathcal{I}_x\mathcal{K}(x,\cdot)\|_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)}\\ &= \left[\int_{\mathcal{B}^d_R}\int_{\mathcal{B}^d_R} \mathcal{K}(x,y)\,\mathrm{d}\sigma^*_d(x)\mathrm{d}\sigma^*_d(y)\right]^{\frac{1}{2}}\\ &= \sqrt{\frac{d}{\omega_d R^d}}\frac{1}{A_{0,0}}. \qquad (6.67)\end{aligned}$$

6.7.2 Tractability of Multivariate Integration

While dealing with higher dimensional problems, a predictable issue is the increase of cost with the increase of dimension d, which is actually the curse of dimensionality. The same issue arises for multivariate integration. Hence, it is reasonable to investigate the tractability of integration in higher dimensions for our particular Sobolev space. Many authors have investigated the tractability of multivariate integration with different function spaces. For further information the reader is referred to [33, 55, 56, 65]. Formally, tractability is interpreted as the existence of a method that approximates the solution with an error using N samples of a function, where N depends on the error and dimension d and is bounded. Based on the worst case error calculated in the previous section, we now define the term tractability.

Definition 6.7.5 *Tractability is the minimal number of function evaluations required to reduce the initial integration error by a factor ε, i.e.*

$$N^{(\varepsilon,d)}_{\min} := \min\left\{N :\, \exists\, \mathcal{Q}_{N,d} \,|\, \mathcal{E}(\mathcal{Q}_{N,d}) \le \varepsilon\cdot\mathcal{E}(\mathcal{Q}_{0,d})\right\}. \qquad (6.68)$$

In addition, we define the tractability for average sample points as follows

$$N^{(\varepsilon,d)}_{\mathrm{avg}} := \min\left\{N :\, \exists\, \mathcal{Q}_{N,d} \,|\, \mathcal{E}^{\mathrm{avg}}(\mathcal{Q}_{N,d}) \le \varepsilon\cdot\mathcal{E}^{\mathrm{avg}}(\mathcal{Q}_{0,d})\right\}, \qquad (6.69)$$

where $\mathcal{E}^{\mathrm{avg}}(\mathcal{Q}_{0,d}) = \mathcal{E}(\mathcal{Q}_{0,d})$ by Definition 6.7.2.

Remark 6.7.6 *Tractability of multivariate integration indicates the existence of at least one cubature rule that is tractable, while tractability of average sample points implies that there exist many cubature rules that are tractable.*

Definition 6.7.7 *The multivariate integration in the Sobolev space $\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)$ is said to be tractable if there exist constants $C, \alpha, \beta \in \mathbb{R}^+$ such that the inequality*

$$N^{(\varepsilon,d)}_{\min} \leq C\, d^{\alpha} \varepsilon^{-\beta} \tag{6.70}$$

holds for all the dimensions $d \geq 3$ and for all $\varepsilon \in (0,1)$. Multivariate integration in the space $\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)$ is said to be strongly tractable if (6.70) holds for $\alpha = 0$. Furthermore, the multivariate integration is said to be tractable for average sample points (see [64]) if and only if there exist $C, \alpha, \beta \in \mathbb{R}^+$ such that

$$N^{(\varepsilon,d)}_{\mathrm{avg}} \leq C\, d^{\alpha} \varepsilon^{-\beta}. \tag{6.71}$$

The minimal values of α and β are called the d-exponent and the ε-exponent of the (strong) tractability, respectively.

Remark 6.7.8 [64]

1. *If the multivariate integration is tractable for average sample points then it is also tractable.*
2. *The ε- and d-exponents of tractability do not exceed the corresponding exponents of tractability for average sample points.*

Theorem 6.7.9 *For $d \geq 3$ and $(m,n,j) \neq (0,0,1)$, we have*

$$\mathbb{E}\left[G^{\mathrm{X},d}_{m,n,j}(x_i) G^{\mathrm{X},d}_{m,n,j}(x_k)\right] = \begin{cases} 0, & i \neq k \\ \frac{d}{\omega_d R^d} & i = k. \end{cases} \tag{6.72}$$

Proof: Using Definition 1.5.4 and Theorem 6.3.1, we calculate the expectation of the orthonormal systems $G^{\mathrm{X},d}_{m,n,j}$ as follows. For the case $i \neq k$, we obtain

$$\begin{aligned}
\mathbb{E}\left[G^{\mathrm{X},d}_{m,n,j}(x_i) G^{\mathrm{X},d}_{m,n,j}(x_k)\right] &= \int_{\mathcal{B}^d_R} \int_{\mathcal{B}^d_R} G^{\mathrm{X},d}_{m,n,j}(x_i) G^{\mathrm{X},d}_{m,n,j}(x_k) \mathrm{d}\sigma^*_d(x_i) \mathrm{d}\sigma^*_d(x_k) \\
&= \int_{\mathcal{B}^d_R} G^{\mathrm{X},d}_{m,n,j}(x_i) \mathrm{d}\sigma^*_d(x_i) \int_{\mathcal{B}^d_R} G^{\mathrm{X},d}_{m,n,j}(x_k) \mathrm{d}\sigma^*_d(x_k) \\
&= 0.
\end{aligned}$$

For $i = k$, we get

$$\begin{aligned}
\mathbb{E}\left[\left(G^{\mathrm{X},d}_{m,n,j}(x_i)\right)^2\right] &= \int_{\mathcal{B}^d_R} \left(G^{\mathrm{X},d}_{m,n,j}(x_i)\right)^2 \mathrm{d}\sigma^*_d(x_i) \\
&= \frac{d}{\omega_d R^d}.
\end{aligned}$$

This completes the proof. ■

In what follows, we discuss the conditions on the d-exponent and ε-exponent that allows the integration to be tractable and strongly tractable in the Sobolev space $\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)$. In this result, we only consider the case of equal weight quadrature rules. The reason is: the term $N_{\min}^{(\varepsilon,d)}$ is smaller for weighted quadrature rules than the one with equal weights, as the quadrature rules with equal weights is a subclass of the weighted quadature rules. And eventually, we also get a bound for the weighted case. As in Theorem 6.7.3, we again use the condition $l_0 = 0$ for the case of type I in the following result.

Theorem 6.7.10 *Integration in the Sobolev space $\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)$ is strongly tractable with the ε-exponent of strong tractability at most equal to 2, if the sequences $\{A_{m,n}(d)\}$, briefly $\{A_{m,n}\}$ satisfy*

$$\limsup_{d} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} A_{m,n}^{-2}\mathcal{Z}(d,n) < +\infty. \tag{6.73}$$

Let

$$\alpha = \limsup_{d} \frac{\ln\left(\sum\limits_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} A_{m,n}^{-2}\mathcal{Z}(d,n)\right)}{\ln d}, \tag{6.74}$$

if $\alpha < +\infty$, integration in the space $\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)$ is tractable with ε-exponent and d-exponent of tractability at most equal to 2 and α, respectively.

Proof: In order to prove tractability, we only need to prove the tractability of average sample points, since from Remark 6.7.8 the ε- and d-exponents for tractability are not greater than the corresponding ones of tractability for average sample points. First, we calculate the expectation of the worst case error, using Theorem 6.7.3, as

$$\begin{aligned}
\mathbb{E}\left[\mathcal{E}(\mathcal{Q}_{N,d})^2\right] &= \mathbb{E}\left[\frac{1}{N^2}\sum_{i,k=1}^{N}\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}}\sum_{j=1}^{\mathcal{Z}(d,n)}\frac{G_{m,n,j}^{\mathrm{X},d}(x_i)G_{m,n,j}^{\mathrm{X},d}(x_k)}{A_{m,n}^2}\right]\\
&= \frac{1}{N^2}\sum_{i,k=1}^{N}\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}}\sum_{j=1}^{\mathcal{Z}(d,n)}\frac{1}{A_{m,n}^2}\mathbb{E}\left[G_{m,n,j}^{\mathrm{X},d}(x_i)G_{m,n,j}^{\mathrm{X},d}(x_k)\right].
\end{aligned}$$

Now, using the expectation of the orthonormal basis systems $G^{\mathrm{X},d}_{m,n,j}$ from Theorem 6.7.9, we obtain

$$\mathbb{E}\left[\mathcal{E}(\mathcal{Q}_{N,d})^2\right] = \frac{1}{N^2} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \sum_{j=1}^{\mathcal{Z}(d,n)} \frac{1}{A^2_{m,n}} \cdot N \cdot \frac{d}{\omega_d R^d}.$$

Having the expectation of $\mathcal{E}(\mathcal{Q}_{N,d})^2$, we can now calculate the value of $\mathcal{E}^{\mathrm{avg}}$. In accordance with Definition 6.7.2, we get

$$\mathcal{E}^{\mathrm{avg}}(\mathcal{Q}_{N,d}) = \left[\frac{1}{N}\frac{d}{\omega_d R^d} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{\mathcal{Z}(d,n)}{A^2_{m,n}}\right]^{\frac{1}{2}}. \tag{6.75}$$

Now, using the definition of tractability for average sample points and equation (6.67), we proceed as follows

$$\begin{aligned}
N^{(\varepsilon,d)}_{\mathrm{avg}} &= \min\{N : \mathcal{E}^{\mathrm{avg}}(\mathcal{Q}_{N,d}) \leq \varepsilon \cdot \mathcal{E}(\mathcal{Q}_{0,d})\} \\
&= \min\left\{N : \left[\frac{1}{N}\frac{d}{\omega_d R^d} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{\mathcal{Z}(d,n)}{A^2_{m,n}}\right]^{\frac{1}{2}} \leq \varepsilon \cdot \frac{1}{A_{0,0}}\sqrt{\frac{d}{\omega_d R^d}}\right\} \\
&= \min\left\{N : \frac{1}{N} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{\mathcal{Z}(d,n)}{A^2_{m,n}} \leq \varepsilon^2 \cdot \frac{1}{A^2_{0,0}}\right\} \\
&= \min\left\{N : \varepsilon^{-2} A^2_{0,0} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{\mathcal{Z}(d,n)}{A^2_{m,n}} \leq N\right\}.
\end{aligned}$$

According to the definition of Gaussian bracket, it is easy to see that the above equation represents the ceiling function for N. Hence, we get

$$N^{(\varepsilon,d)}_{\mathrm{avg}} = \left\lceil \varepsilon^{-2} A^2_{0,0} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} \frac{\mathcal{Z}(d,n)}{A^2_{m,n}} \right\rceil.$$

By the mean value theorem of integration, we can find a sample of N points for which $\mathcal{E}(\mathcal{Q}_{N,d}) \le \mathcal{E}^{\mathrm{avg}}(\mathcal{Q}_{N,d})$ and consequently, we get

$$N_{\min}^{(\varepsilon,d)} \le \left\lceil \varepsilon^{-2} A_{0,0}^2 \sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} \frac{\mathcal{Z}(d,n)}{A_{m,n}^2} \right\rceil,$$

which implies

$$N_{\min}^{(\varepsilon,d)} \le \varepsilon^{-2} A_{0,0}^2 \sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} \frac{\mathcal{Z}(d,n)}{A_{m,n}^2}. \tag{6.76}$$

As stated in Definition 6.7.7, this indicates that the strong tractability of integration in $\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)$ holds for $\beta = 2$ and $C = A_{0,0}^2 \sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} \frac{\mathcal{Z}(d,n)}{A_{m,n}^2}$, if

$$\limsup_{d} \sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} A_{m,n}^{-2} \mathcal{Z}(d,n) < +\infty.$$

Furthermore, we suppose $u := \sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} A_{m,n}^{-2} \mathcal{Z}(d,n)$, which implies

$$\begin{aligned} \ln u &= \frac{\ln\left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} A_{m,n}^{-2} \mathcal{Z}(d,n) \right)}{\ln d} \cdot \ln d \\ &= \ln d^{\frac{\ln\left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} A_{m,n}^{-2} \mathcal{Z}(d,n) \right)}{\ln d}}. \end{aligned}$$

Consequently, we get

$$u = d^{\frac{\ln\left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} A_{m,n}^{-2} \mathcal{Z}(d,n) \right)}{\ln d}}.$$

This in turn suggests that (6.76) can be rewritten as follows

$$N_{\min}^{(\varepsilon,d)} \le \varepsilon^{-2} A_{0,0}^2\, d^{\frac{\ln\left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n\ge 0}} A_{m,n}^{-2} \mathcal{Z}(d,n) \right)}{\ln d}}, \tag{6.77}$$

indicating tractability of integration in $\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)$ for $\beta = 2$, $C = A_{0,0}^2$ and

$$\alpha = \limsup_{d} \frac{\ln\left(\sum_{\substack{(m,n)\neq(0,0)\\ l_n\geq 0}} A_{m,n}^{-2}\mathcal{Z}(d,n)\right)}{\ln d},$$

with $\alpha < +\infty$. ■

6.7.3 Diaphony

The convergence of the generalized discrepancy (2.17) is already discussed in Chapter 5 for uniformly distributed i.i.d. random variables. In this section, we will discuss the convergence of the generalized discrepancy using a different approach. Since, in general the generalized discrepancy depends on the reproducing kernel and then consequently on the Sobolev space $\mathcal{H}_{s,t}^{\mathrm{X},d}$, we need to find the assumptions or conditions on $\mathcal{H}_{s,t}^{\mathrm{X},d}$ or the reproducing kernel $\mathcal{K}$ such that the generalized discrepancy converges for a uniformly distributed set of points as $N \to \infty$. Firstly, we present briefly the concepts of G-uniform distribution and G-diaphony. These notions and the corresponding definitions were introduced in [3] and were applied for the spherical settings in [12]. In the following results, we apply these concepts to the case of a d-dimensional ball for our specific settings.

Definition 6.7.11 *Let $\mathcal{H}_{s,t}^{\mathrm{X},d}$ be the Sobolev space on $\mathcal{B}_R^d$ defined by Definition 6.5.4, with the reproducing kernel $\mathcal{K} := \mathcal{K}_{\mathcal{H}_{s,t}^{\mathrm{X},d}}$. A sequence of points $\{x_i\}_{i\geq 1}$ on $\mathcal{B}_R^d$ is said to be G-uniformly distributed if*

$$\lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} F(x_i) = \langle F, G\rangle_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)} \quad \text{for every } F \in \mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d), \tag{6.78}$$

where G is a fixed element of $\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)$.

Definition 6.7.12 *For every $N \geq 1$, let*

$$r_N := \frac{1}{N}\sum_{i=1}^{N} \mathcal{K}(\cdot, x_i) - G. \tag{6.79}$$

Then $\|r_N\|_{\mathcal{H}_{s,t}^{\mathrm{X},d}(\mathcal{B}_R^d)}$ is called the G-diaphony of $\{x_i\}_{i\geq 1}$ and $\|r_N\|_\infty := \sup_{x\in\mathcal{B}_R^d} |r_N(x)|$ is called the G-discrepancy of $\{x_i\}_{i\geq 1}$.

Remark 6.7.13 *For all* $F \in \mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)$,

$$\left| \frac{1}{N} \sum_{i=1}^{N} F(x_i) - \langle F, G \rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} \right| \leq \|F\|_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} \|r_N\|_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} . \tag{6.80}$$

Proof: Using the property (2) of a reproducing kernel $\mathcal{K}$ from Definition 1.1.14, we get the following equation:

$$\left| \frac{1}{N} \sum_{i=1}^{N} F(x_i) - \langle F, G \rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} \right| = \left| \frac{1}{N} \sum_{i=1}^{N} \langle F, \mathcal{K}(\cdot, x_i) \rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} - \langle F, G \rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} \right| .$$

Further, in accordance with equation (6.79) and the bilinearity of the inner product, we get

$$\begin{aligned} \left| \frac{1}{N} \sum_{i=1}^{N} F(x_i) - \langle F, G \rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} \right| &= \left| \left\langle F, \frac{1}{N} \sum_{i=1}^{N} \mathcal{K}(\cdot, x_i) - G \right\rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} \right| \\ &= \left| \langle F, r_N \rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} \right| . \end{aligned} \tag{6.81}$$

Finally, the Cauchy-Schwarz inequality (1.17) allows us to arrive at the result

$$\left| \frac{1}{N} \sum_{i=1}^{N} F(x_i) - \langle F, G \rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} \right| \leq \|F\|_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} \|r_N\|_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} .$$

■

A result similar to the following theorem for G-uniformly distributed sequences on a compact set $E = [0, 1[^s$ and its proof are stated in [3].

Theorem 6.7.14 *A sequence of points* $\{x_i\}_{i \geq 1}$ *on* $\mathcal{B}^d_R$ *is* G*-uniformly distributed if and only if*

$$\lim_{N \to \infty} \|r_N\|_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} = 0. \tag{6.82}$$

Proof: First, we consider that $\{x_i\}_{i \geq 1}$ is G-uniformly distributed, then by Definition 6.7.11, for $F \in \mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)$, we have

$$\lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} F(x_i) = \langle F, G \rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)}.$$

Since $\mathcal{K}$ is a reproducing kernel, then for $\mathcal{K}(x, \cdot) \in \mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)$ and for all $x \in \mathcal{B}^d_R$, we can write

$$\lim_{N \to \infty} \left\langle F, \frac{1}{N} \sum_{i=1}^{N} \mathcal{K}(\cdot, x_i) - G \right\rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} = 0.$$

This yields

$$\lim_{N\to\infty} \langle F, r_N\rangle_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)} = 0.$$

This gives us the weak convergence of r_N as $N \to \infty$, where $\{r_N\}_{N\geq 1}$ is a sequence of continuous functions (see Lemma 6.5.3). Since every weakly convergent sequence on a compact set converges uniformly ([3]), we obtain the uniform convergence of r_N, i.e.

$$\|r_N\|_\infty = \sup_{x\in\mathcal{B}^d_R} |r_N(x)| \xrightarrow[N\to\infty]{} 0. \tag{6.83}$$

Now consider the norm of r_N in $\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)$

$$\begin{aligned}
0 &\leq \|r_N\|^2_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)} \\
&= \left\langle \frac{1}{N}\sum_{i=1}^N \mathcal{K}(x_i,\cdot) - G, \frac{1}{N}\sum_{k=1}^N \mathcal{K}(x_k,\cdot) - G \right\rangle_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)} \\
&= \frac{1}{N}\sum_{i=1}^N \frac{1}{N}\sum_{k=1}^N \langle \mathcal{K}(x_i,\cdot), \mathcal{K}(x_k,\cdot)\rangle_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)} - \frac{1}{N}\sum_{i=1}^N \langle \mathcal{K}(x_i,\cdot), G\rangle_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)} \\
&\qquad - \frac{1}{N}\sum_{k=1}^N \langle G, \mathcal{K}(x_k,\cdot)\rangle_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)} + \langle G, G\rangle_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)}.
\end{aligned}$$

Using Definition 1.1.14, the above equation takes the following form:

$$\begin{aligned}
&\|r_N\|^2_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)} \\
&= \left| \frac{1}{N}\sum_{i=1}^N \frac{1}{N}\sum_{k=1}^N \mathcal{K}(x_i,x_k) - \frac{1}{N}\sum_{i=1}^N \langle G, \mathcal{K}(x_i,\cdot)\rangle_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)} - \frac{1}{N}\sum_{k=1}^N G(x_k) \right. \\
&\qquad \left. + \langle G, G\rangle_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)} \right| \\
&\leq \frac{1}{N}\sum_{k=1}^N \left| \frac{1}{N}\sum_{i=1}^N \mathcal{K}(x_i,x_k) - G(x_k)\right| + \left| \frac{1}{N}\sum_{i=1}^N G(x_i) - \|G\|^2_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)}\right| \\
&= \frac{1}{N}\sum_{k=1}^N |r_N(x_k)| + \left| \frac{1}{N}\sum_{i=1}^N G(x_i) - \|G\|^2_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)}\right| \\
&\leq \sup_{x\in\mathcal{B}^d_R} |r_N(x)| + \left| \frac{1}{N}\sum_{i=1}^N G(x_i) - \|G\|^2_{\mathcal{H}^{X,d}_{s,t}(\mathcal{B}^d_R)}\right|.
\end{aligned} \tag{6.84}$$

Now from equation (6.83), the first part of (6.84) converges uniformly to zero as N approaches infinity. Also by our assumption, $\{x_i\}_{i\geq 1}$ is G-uniformly distributed so the second part of (6.84) also converges to zero as N approaches infinity. This implies

$$\|r_N\|_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} \xrightarrow[N\to\infty]{} 0.$$

Conversely, suppose that (6.82) holds true. Now using the Cauchy-Schwarz inequality (1.17), the convergence of $\|r_N\|$ in $\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)$ guarantees the weak convergence of r_N and hence, for all $F \in \mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)$, we get

$$\lim_{N\to\infty} \langle r_N, F\rangle_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} = 0.$$

The above equation, together with the equation (6.81), leads us to the required result. ■

Theorem 6.7.15 *Let $\mathcal{P}_N$ be a sequence of N points on $\mathcal{B}^d_R$, i.e. $\mathcal{P}_N = \{x_1, x_2, \ldots, x_N\} \subset \mathcal{B}^d_R$, then for a pseudodifferential operator $\mathcal{A}$ on $\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)$ satisfying the conditions stated in Theorem 6.6.1 and a fixed function $G \in \mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)$, the following equality holds*

$$\|r_N\|^2_{\mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)} = D^2(\mathcal{P}_N, \mathcal{A}). \tag{6.85}$$

For the type $\mathrm{X} = \mathrm{I}$, we require a sufficient condition of $l_0 = 0$.

Proof: We first consider the case for type $\mathrm{X} = \mathrm{II}$. We choose a constant function $G = \frac{d}{\omega_d R^d}\frac{1}{A^2_{0,0}}$. Since the eigenvalues $A_{0,0}$ are non-vanishing, $G \in \mathcal{H}^{\mathrm{II},d}_{s,t}(\mathcal{B}^d_R)$. From Definition 6.7.12, we have

$$r_N(x) = \frac{1}{N}\sum_{k=1}^{N}\left[\sum_{\substack{m,n=0\\A_{m,n}\neq 0}}^{\infty}\sum_{j=1}^{\mathcal{Z}(d,n)} \frac{1}{A^2_{m,n}} G^{\mathrm{II},d}_{m,n,j}(x_k) G^{\mathrm{II},d}_{m,n,j}(x)\right] - \frac{d}{\omega_d R^d}\frac{1}{A^2_{0,0}}.$$

The convergence of the infinite summation in the above equation allows us to interchange the summations.

$$\begin{aligned} r_N(x) &= \sum_{\substack{m,n=0\\A_{m,n}\neq 0}}^{\infty}\sum_{j=1}^{\mathcal{Z}(d,n)} \frac{1}{A^2_{m,n}}\left[\frac{1}{N}\sum_{k=1}^{N} G^{\mathrm{II},d}_{m,n,j}(x_k)\right] G^{\mathrm{II},d}_{m,n,j}(x) - \frac{d}{\omega_d R^d}\frac{1}{A^2_{0,0}} \\ &= \sum_{\substack{(m,n)\neq(0,0)\\A_{m,n}\neq 0}}\sum_{j=1}^{\mathcal{Z}(d,n)} \frac{1}{A^2_{m,n}}\left[\frac{1}{N}\sum_{k=1}^{N} G^{\mathrm{II},d}_{m,n,j}(x_k)\right] G^{\mathrm{II},d}_{m,n,j}(x). \end{aligned}$$

This gives us the inner product of r_N with $G^{\mathrm{II},d}_{m,n,j}$ as follows

$$\left\langle r_N, G^{\mathrm{II},d}_{m,n,j} \right\rangle_{\mathrm{L}^2(\mathcal{B}^d_R)} = \frac{1}{A^2_{m,n}} \left[\frac{1}{N} \sum_{k=1}^{N} G^{\mathrm{II},d}_{m,n,j}(x_k) \right]$$

for all $(m,n) \neq (0,0)$. Also, the norm of r_N in $\mathcal{H}^{\mathrm{II},d}_{s,t}(\mathcal{B}^d_R)$ from the definition of the Sobolev space (see Definition 6.5.1) is given by

$$\|r_N\|^2_{\mathcal{H}^{\mathrm{II},d}_{s,t}(\mathcal{B}^d_R)} = \sum_{m,n=0}^{\infty} \sum_{j=1}^{\mathcal{Z}(d,n)} A^2_{m,n} \left\langle r_N, G^{\mathrm{II},d}_{m,n,j} \right\rangle^2_{\mathrm{L}^2(\mathcal{B}^d_R)}.$$

Further, separating the $(m,n) = (0,0)$-term and using the fact that for our chosen G

$$\left\langle r_N, G^{\mathrm{II},d}_{m,n,j} \right\rangle^2_{\mathrm{L}^2(\mathcal{B}^d_R)} = 0 \quad \text{for } m = n = 0,$$

we see that

$$\begin{aligned}
\|r_N\|^2_{\mathcal{H}^{\mathrm{II},d}_{s,t}(\mathcal{B}^d_R)} &= A^2_{0,0} \left\langle r_N, G^{\mathrm{II},d}_{0,0,1} \right\rangle^2_{\mathrm{L}^2(\mathcal{B}^d_R)} + \sum_{(m,n)\neq(0,0)} \sum_{j=1}^{\mathcal{Z}(d,n)} A^2_{m,n} \left\langle r_N, G^{\mathrm{II},d}_{m,n,j} \right\rangle^2_{\mathrm{L}^2(\mathcal{B}^d_R)} \\
&= \frac{1}{N^2} \sum_{\substack{(m,n)\neq(0,0) \\ A_{m,n}\neq 0}} \sum_{j=1}^{\mathcal{Z}(d,n)} \sum_{i,k=1}^{N} \frac{1}{A^2_{m,n}} G^{\mathrm{II},d}_{m,n,j}(x_k) G^{\mathrm{II},d}_{m,n,j}(x_i) \\
&= D^2(\mathcal{P}_N, \mathrm{II}, \mathcal{A}).
\end{aligned}$$

Next, for the type $\mathrm{X} = \mathrm{I}$, we use the condition on l_n, i.e. $l_0 = 0$ for $n = 0$ and $l_n \geq 0$ for all $n \in \mathbb{N}$. We again choose $G = \frac{d}{\omega_d R^d} \frac{1}{A^2_{0,0}} \in \mathcal{H}^{\mathrm{I},d}_{s,t}(\mathcal{B}^d_R)$. Analogous calculations enable us to conclude

$$\|r_N\|^2_{\mathcal{H}^{\mathrm{I},d}_{s,t}(\mathcal{B}^d_R)} = D^2(\mathcal{P}_N, \mathrm{I}, \mathcal{A}).$$

This proves the result. ■

Remark 6.7.16 *Note that for $l_n = n$, we do not have to restrict the value of l_0 in the proof of Theorem 6.7.15, as the choice of the function $G \in \mathcal{H}^{\mathrm{X},d}_{s,t}(\mathcal{B}^d_R)$ is the same for the type* I *and the* II *cases.*

Chapter 7

Numerical Tests: Numerical Integration

In practical applications, we often come across with the problems in geosciences, where the integral of the function has to be evaluated on the domain of a ball. However, usually either the integral is difficult or impossible to evaluate or the integrand is not known continuously over the domain but only at specific points. These situations lead to approximate integration. In this chapter, we consider particular examples for the theory of approximate integration on a ball and its application. In addition, we discuss the outcomes.

We know that the discrepancy formula (2.17) originates from the error bound of the cubature rule (2.15). Hence, minimal-discrepancy point grids guarantee a good approximation for the integration of functions on the ball. For the numerical implementation of this concept and in order to observe how good our grids approximate the integrals on the ball, we proceed as follows: we choose the product of orthonormal system II

$$x \mapsto \left(G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}\right)(x), \quad x \in \mathcal{B}$$

as our function for $m, n, m_1, n_1 \in \mathbb{N}_0$ and $j \in \{1, 2, \ldots, 2n+1\}$, $j_1 \in \{1, 2, \ldots, 2n_1 + 1\}$, whose integral has to be evaluated on a 3-dimensional unit ball $\mathcal{B}$. Then, Theorem 1.4.1 implies that

$$\int_{\mathcal{B}} G^{\mathrm{II}}_{m,n,j}(x) G^{\mathrm{II}}_{m_1,n_1,j_1}(x)\,\mathrm{d}x = \delta_{mm_1}\delta_{nn_1}\delta_{jj_1}. \tag{7.1}$$

Having an exact value of the integral, we can now check the performance of our grids generated on the ball. With the help of quadrature formula (2.15), we approximate the integral in (7.1) as

$$\int_{\mathcal{B}} \left(G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}\right)(x)\,\mathrm{d}x \approx \frac{4\pi}{3N} \sum_{k=1}^{N} \left(G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}\right)(x_k). \tag{7.2}$$

Using (2.16) for our chosen function, we get the following inequality for the error estimate of the quadrature rule (7.2):

$$\begin{aligned} &\left| \frac{3}{4\pi} \int_{\mathcal{B}} G^{\mathrm{II}}_{m,n,j}(x) G^{\mathrm{II}}_{m_1,n_1,j_1}(x)\,\mathrm{d}x - \frac{1}{N} \sum_{k=1}^{N} G^{\mathrm{II}}_{m,n,j}(x_k) G^{\mathrm{II}}_{m_1,n_1,j_1}(x_k) \right| \\ &\qquad \leq \left\| \mathcal{A}\left(G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}\right) \right\|_{\mathrm{L}^2(\mathcal{B})} \times D\left(\omega_N, \mathcal{A}\right), \end{aligned} \tag{7.3}$$

where $\mathcal{A}$ is pseudodifferential operator satisfying the conditions in Theorem 2.2.1 with summable eigenvalues $\{A_{m,n}\}_{m,n\in\mathbb{N}_0}$ and ω_N is a set of points on $\mathcal{B}$. In order to calculate the upper bound of this cubature error, apart from the discrepancy estimate $D\left(\omega_N, \mathcal{A}\right)$, we also require to compute the norm $\left\| \mathcal{A}\left(G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}\right) \right\|$ in the $\mathrm{L}^2(\mathcal{B})$-space. The Parseval's identity (1.25) and the self-adjoint property of the operator $\mathcal{A}$ allow us to write

$$\begin{aligned} \left\| \mathcal{A}\left(G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}\right) \right\|^2_{\mathrm{L}^2(\mathcal{B})} &= \sum_{m_2,n_2=0}^{\infty} \sum_{j_2=1}^{2n_2+1} \left\langle \mathcal{A}\left(G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}\right), G^{\mathrm{II}}_{m_2,n_2,j_2} \right\rangle^2_{\mathrm{L}^2(\mathcal{B})} \\ &= \sum_{m_2,n_2=0}^{\infty} \sum_{j_2=1}^{2n_2+1} \left\langle G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}, \mathcal{A} G^{\mathrm{II}}_{m_2,n_2,j_2} \right\rangle^2_{\mathrm{L}^2(\mathcal{B})}. \end{aligned} \tag{7.4}$$

Next, we consider the inner product in the above sum

$$\left\langle G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}, \mathcal{A} G^{\mathrm{II}}_{m_2,n_2,j_2} \right\rangle_{\mathrm{L}^2(\mathcal{B})} = \int_{\mathcal{B}} G^{\mathrm{II}}_{m,n,j}(x) G^{\mathrm{II}}_{m_1,n_1,j_1}(x) \mathcal{A} G^{\mathrm{II}}_{m_2,n_2,j_2}(x)\mathrm{d}x.$$

With $\mathcal{A} G^{\mathrm{II}}_{m_2,n_2,j_2} = A_{m_2,n_2} G^{\mathrm{II}}_{m_2,n_2,j_2}$, we arrive at

$$\begin{aligned} &\left\langle G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}, \mathcal{A} G^{\mathrm{II}}_{m_2,n_2,j_2} \right\rangle_{\mathrm{L}^2(\mathcal{B})} \\ &\qquad = A_{m_2,n_2} \int_{\mathcal{B}} G^{\mathrm{II}}_{m,n,j}(x) G^{\mathrm{II}}_{m_1,n_1,j_1}(x) G^{\mathrm{II}}_{m_2,n_2,j_2}(x)\mathrm{d}x. \end{aligned} \tag{7.5}$$

Using the definition of the orthonormal system II given by (1.51) and Theorem 1.1.25, we obtain

$$\begin{aligned} &\left\langle G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}, \mathcal{A} G^{\mathrm{II}}_{m_2,n_2,j_2} \right\rangle_{\mathrm{L}^2(\mathcal{B})} \\ &= A_{m_2,n_2} \sqrt{(2m+3)(2m_1+3)(2m_2+3)} \int_0^1 \int_{\Omega} P^{(0,2)}_{m}(2r-1) P^{(0,2)}_{m_1}(2r-1) \\ &\qquad \times P^{(0,2)}_{m_2}(2r-1) Y_{n,j}(\xi) Y_{n_1,j_1}(\xi) Y_{n_2,j_2}(\xi)\, r^2 \,\mathrm{d}\omega(\xi)\,\mathrm{d}r. \end{aligned} \tag{7.6}$$

This left us to solve two integrals, that are:

$$\int_0^1 r^2 P_m^{(0,2)}(2r-1)P_{m_1}^{(0,2)}(2r-1)P_{m_2}^{(0,2)}(2r-1)\,\mathrm{d}r \tag{7.7}$$

and

$$\int_\Omega Y_{n,j}(\xi)Y_{n_1,j_1}(\xi)Y_{n_2,j_2}(\xi)\,\mathrm{d}\omega(\xi). \tag{7.8}$$

For calculating the first integral, we substitute

$$t = 2r-1$$

with $\mathrm{d}r = \frac{\mathrm{d}t}{2}$ in (7.7) and obtain

$$\frac{1}{8}\int_{-1}^1 (1+t)^2 P_m^{(0,2)}(t)P_{m_1}^{(0,2)}(t)P_{m_2}^{(0,2)}(t)\,\mathrm{d}t. \tag{7.9}$$

Now, we use the Gauss-Jacobi quadrature (see [39]) on the interval $[-1,1]$, i.e.

$$\int_{-1}^1 (1-t)^\alpha(1+t)^\beta g(t)\,\mathrm{d}t \approx \sum_{i=1}^M w_i g(t_i) \tag{7.10}$$

for a function $g:[-1,1]\to\mathbb{R}$, to obtain an approximation of the integral in (7.9) with the parameters $\alpha=0$ and $\beta=2$ as

$$\int_{-1}^1 (1-t)^0(1+t)^2 P_m^{(0,2)}(t)P_{m_1}^{(0,2)}(t)P_{m_2}^{(0,2)}(t)\,\mathrm{d}t$$
$$\approx \sum_{i=1}^M w_i P_m^{(0,2)}(t_i)P_{m_1}^{(0,2)}(t_i)P_{m_2}^{(0,2)}(t_i). \tag{7.11}$$

The weights w_i in (7.10) are given as

$$w_i = \frac{2M+\alpha+\beta+2}{M+\alpha+\beta+1}\frac{\Gamma(M+\alpha+1)}{\Gamma(M+\alpha+\beta+1)}\frac{\Gamma(M+\beta+1)}{(M+1)!}\frac{2^{\alpha+\beta}}{P_M^{(\alpha,\beta)\prime}(t_i)P_{M+1}^{(\alpha,\beta)}(t_i)}, \tag{7.12}$$

where $P_M^{(\alpha,\beta)\prime}$ denotes the first order derivative of $P_M^{(\alpha,\beta)}$ and t_i's are the zeros of Jacobi polynomials of degree M, i.e. $P_M^{(\alpha,\beta)}$. Using equation (1.35) with the parameters $\alpha=0$, $\beta=2$, we have

$$P_M^{(0,2)\prime}(t) = \frac{\mathrm{d}}{\mathrm{d}t}P_M^{(0,2)}(t) = \frac{M+3}{2}P_{M-1}^{(1,3)}(t). \tag{7.13}$$

As a result, (7.12) yields the weights for the approximation in (7.11), that are:

$$w_i = \frac{M+2}{(M+1)(M+3)^2} \frac{16}{P_{M-1}^{(1,3)}(t_i) P_{M+1}^{(0,2)}(t_i)}. \tag{7.14}$$

Thus, (7.9) yields

$$\frac{1}{8}\int_{-1}^{1} (1+t)^2 P_m^{(0,2)}(t) P_{m_1}^{(0,2)}(t) P_{m_2}^{(0,2)}(t)\,\mathrm{d}t$$
$$\approx \sum_{i=1}^{M} \frac{2(M+2)}{(M+1)(M+3)^2} \frac{P_m^{(0,2)}(t_i) P_{m_1}^{(0,2)}(t_i) P_{m_2}^{(0,2)}(t_i)}{P_{M-1}^{(1,3)}(t_i) P_{M+1}^{(0,2)}(t_i)}, \tag{7.15}$$

where the roots t_i of the Jacobi polynomials are computed using the Newton-Raphson Method.

We note that the integral in (7.15), as a result of the orthogonality property of the Jacobi polynomials, vanishes for all degrees $m_2 > m + m_1$. Hence, if we choose t_i zeros of $P_{m_2}^{(0,2)}$ for $i = 1, 2, \ldots, m_2$, then there exist weights w_i for $i = 1, 2, \ldots, m_2$ which make the Gaussian quadrature (7.15) exact for all polynomials of degree less or equal $2m_2 - 1$.

Next, we consider the integral in (7.8). We have a nice expression for the integral over a product of three spherical harmonics (see [18]), i.e.

$$\int_\Omega Y_{n,j}(\xi) Y_{n_1,j_1}(\xi) Y_{n_2,j_2}(\xi) \mathrm{d}\omega(\xi)$$
$$= \left[\frac{(2n+1)(2n_1+1)(2n_2+1)}{4\pi}\right]^{\frac{1}{2}} \begin{pmatrix} n & n_1 & n_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} n & n_1 & n_2 \\ j & j_1 & j_2 \end{pmatrix}, \tag{7.16}$$

where $\begin{pmatrix} n & n_1 & n_2 \\ j & j_1 & j_2 \end{pmatrix}$ denotes the Wigner $3j$-symbol.

Remark 7.0.1 *For the computation of the Wigner $3j$-symbol, we use the result from [73].*

(i) The Wigner $3j$-symbol $\begin{pmatrix} n & n_1 & n_2 \\ j & j_1 & j_2 \end{pmatrix}$ vanishes unless it satisfies the following conditions:

(a) $j \in \{-|n|, \ldots, |n|\}$, $j_1 \in \{-|n_1|, \ldots, |n_1|\}$ and $j_2 \in \{-|n_2|, \ldots, |n_2|\}$,

(b) $j + j_1 + j_2 = 0$,

(c) $|n_1 - n_2| \leq n \leq |n_1 + n_2|$,

(d) $n + n_1 + n_2 \in \mathbb{Z}$.

(ii) The Wigner 3j-symbol is calculated as

$$
\begin{aligned}
&\begin{pmatrix} n & n_1 & n_2 \\ j & j_1 & j_2 \end{pmatrix} \\
&\quad = \Delta(n, n_1, n_2)\, \delta_{j+j_1+j_2,0}\, (-1)^{n-n_1-j_2} \\
&\qquad \times \sqrt{(n+j)!\,(n-j)!\,(n_1+j_1)!\,(n_1-j_1)!\,(n_2+j_2)!\,(n_2-j_2)!} \\
&\qquad \times \sum_{k=k_{\min}}^{k_{\max}} \frac{(-1)^k}{k!\,(n+n_1-n_2-k)!\,(n-j-k)!\,(n_1+j_1-k)!} \\
&\qquad \times \frac{1}{(n_2-n_1+j+k)!\,(n_2-n-j_1+k)!},
\end{aligned}
$$

where

$$
\Delta(n, n_1, n_2) = \sqrt{\frac{(n+n_1-n_2)!\,(n-n_1+n_2)!\,(-n+n_1+n_2)!}{(n+n_1+n_2+1)!}},
$$

and

$$
\begin{aligned}
k_{\min} &= \max\{-n_2+n_1-j; -n_2+n+j_1; 0\}, \\
k_{\max} &= \min\{n+n_1-n_2; n-j; n_1+j_1\}.
\end{aligned}
$$

As a result of the above considerations, we can now calculate the inner product in (7.6). Using (7.15) and (7.16), equation (7.6) yields

$$
\begin{aligned}
&\left\langle G^{\mathrm{II}}_{m,n,j} G^{\mathrm{II}}_{m_1,n_1,j_1}, \mathcal{A} G^{\mathrm{II}}_{m_2,n_2,j_2} \right\rangle_{\mathrm{L}^2(\mathcal{B})} \\
&\quad = A_{m_2,n_2} \sqrt{(2m+3)(2m_1+3)(2m_2+3)} \\
&\qquad \times \sum_{i=1}^{M} \left[\frac{2(M+2)}{(M+1)(M+3)^2} \frac{P^{(0,2)}_{m}(t_i) P^{(0,2)}_{m_1}(t_i) P^{(0,2)}_{m_2}(t_i)}{P^{(1,3)}_{M-1}(t_i) P^{(0,2)}_{M+1}(t_i)} \right] \\
&\qquad \times \left[\frac{(2n+1)(2n_1+1)(2n_2+1)}{4\pi} \right]^{\frac{1}{2}} \begin{pmatrix} n & n_1 & n_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} n & n_1 & n_2 \\ j & j_1 & j_2 \end{pmatrix}.
\end{aligned}
$$

The exactness of Gauss-Jacobi quadrature (7.15) and the computation conditions for Wigner 3j-symbol (see Remark 7.0.1) give us a finite sum over m_2

and n_2 in (7.4). As a consequence, we get

$$\begin{aligned}
&\left\|\mathcal{A}\left(G^{\mathrm{II}}_{m,n,j}G^{\mathrm{II}}_{m_1,n_1,j_1}\right)\right\|^2_{\mathrm{L}^2(\mathcal{B})}\\
&= \sum_{m_2=0}^{m+m_1}\sum_{n_2=0}^{n+n_1}\sum_{j_2=1}^{2n_2+1} \frac{(2m+3)(2m_1+3)(2m_2+3)(2n+1)(2n_1+1)(2n_2+1)}{\pi}\\
&\qquad \times A^2_{m_2,n_2}\left[\sum_{i=1}^{M}\frac{M+2}{(M+1)(M+3)^2}\frac{P^{(0,2)}_m(t_i)P^{(0,2)}_{m_1}(t_i)P^{(0,2)}_{m_2}(t_i)}{P^{(1,3)}_{M-1}(t_i)P^{(0,2)}_{M+1}(t_i)}\right]^2\\
&\qquad \times\left[\begin{pmatrix} n & n_1 & n_2\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} n & n_1 & n_2\\ j & j_1 & j_2\end{pmatrix}\right]^2 .
\end{aligned} \tag{7.17}$$

We use here the pseudodifferential operator $\mathcal{A} = \mathbb{A}^{p,q}_{\mathrm{II}}$ with eigenvalues

$$A_{m_2,n_2} = \begin{cases} \left(m_2+\frac{3}{2}\right)^{2q}, & n=0,\ m\in\mathbb{N}_0\\ \left(m_2+\frac{3}{2}\right)^{2q}\left[(2n_2+1)n_2(n_2+1)\right]^p, & n\in\mathbb{N},\ m\in\mathbb{N}_0. \end{cases} \tag{7.18}$$

from Theorem 2.1.3. Note that we used these eigenvalues in Chapter 3 for calculating the discrepancies with parameters $p=\frac{1}{2}$ and $q=\frac{3}{4}$. For numerical calculations, we use here again the same values of p and q.
Moreover, in order to calculate the quadrature error we take a grid of 12, 104 points with a discrepancy estimate 0.0546 on the ball and calculate the approximation error for our chosen function up to degrees $m=m_1=3$ and $n=n_1=1$. Since the Gauss-Jacobi quadrature is exact and hence vanishes for $m_2 > m+m_1$, we can take $M=8$. As a consequence, the sum in (7.17) also vanishes for $m_2 > m+m_1$. Using these considerations, we calculate the norm in (7.17).
The calculated approximation errors, i.e.

$$\left|\frac{3}{4\pi}\int_{\mathcal{B}} G^{\mathrm{II}}_{m,n,j}(x)G^{\mathrm{II}}_{m_1,n_1,j_1}(x)\,\mathrm{d}x - \frac{1}{N}\sum_{k=1}^{N} G^{\mathrm{II}}_{m,n,j}(x_k)G^{\mathrm{II}}_{m_1,n_1,j_1}(x_k)\right|$$

for the selected degrees, are shown in Table 7.1 and the corresponding bounds

$$\left\|\mathbb{A}^{p,q}_{\mathrm{II}}\left(G^{\mathrm{II}}_{m,n,j}G^{\mathrm{II}}_{m_1,n_1,j_1}\right)\right\|_{\mathrm{L}^2(\mathcal{B})} D\left(\omega_N,\mathbb{A}^{p,q}_{\mathrm{II}}\right)$$

are given in Table 7.2. We can see from these computations that the chosen grid gives a good approximation of the integral on the ball. On the other hand, the error bounds for these approximations are increasing with the increasing degree of our chosen function. It stems from the fact that the

Table 7.1: Approximation errors

	$G^{II}_{0,0,0}$	$G^{II}_{1,0,0}$	$G^{II}_{2,0,0}$	$G^{II}_{3,0,0}$	$G^{II}_{0,1,-1}$	$G^{II}_{1,1,-1}$	$G^{II}_{2,1,-1}$	$G^{II}_{3,1,-1}$	$G^{II}_{0,1,0}$	$G^{II}_{1,1,0}$	$G^{II}_{2,1,0}$	$G^{II}_{3,1,0}$	$G^{II}_{0,1,1}$	$G^{II}_{1,1,1}$	$G^{II}_{2,1,1}$	$G^{II}_{3,1,1}$
$G^{II}_{0,0,0}$	0.00	0.04	0.05	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$G^{II}_{1,0,0}$	0.04	0.02	0.07	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$G^{II}_{2,0,0}$	0.05	0.07	0.06	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$G^{II}_{3,0,0}$	0.07	0.09	0.12	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$G^{II}_{0,1,-1}$	0.00	0.00	0.00	0.00	0.00	0.04	0.05	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$G^{II}_{1,1,-1}$	0.00	0.00	0.00	0.00	0.04	0.02	0.07	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$G^{II}_{2,1,-1}$	0.00	0.00	0.00	0.00	0.05	0.07	0.06	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$G^{II}_{3,1,-1}$	0.00	0.00	0.00	0.00	0.07	0.09	0.12	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$G^{II}_{0,1,0}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.05	0.07	0.00	0.00	0.00	0.00
$G^{II}_{1,1,0}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.02	0.07	0.09	0.00	0.00	0.00	0.00
$G^{II}_{2,1,0}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.07	0.06	0.12	0.00	0.00	0.00	0.00
$G^{II}_{3,1,0}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.07	0.09	0.12	0.11	0.00	0.00	0.00	0.00
$G^{II}_{0,1,1}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.05	0.07
$G^{II}_{1,1,1}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.02	0.07	0.09
$G^{II}_{2,1,1}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.07	0.06	0.12
$G^{II}_{3,1,1}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.07	0.09	0.12	0.11

Table 7.2: Error bounds

	$G^{II}_{0,0,0}$	$G^{II}_{1,0,0}$	$G^{II}_{2,0,0}$	$G^{II}_{3,0,0}$	$G^{II}_{0,1,-1}$	$G^{II}_{1,1,-1}$	$G^{II}_{2,1,-1}$	$G^{II}_{3,1,-1}$	$G^{II}_{0,1,0}$	$G^{II}_{1,1,0}$	$G^{II}_{2,1,0}$	$G^{II}_{3,1,0}$	$G^{II}_{0,1,1}$	$G^{II}_{1,1,1}$	$G^{II}_{2,1,1}$	$G^{II}_{3,1,1}$
$G^{II}_{0,0,0}$	0.04	0.10	0.17	0.25	0.18	0.40	0.67	0.98	0.26	0.57	0.95	1.39	0.18	0.40	0.67	0.98
$G^{II}_{1,0,0}$	0.10	0.22	0.38	0.56	0.40	0.88	1.48	2.59	3.90	0.95	2.09	3.08	0.40	0.88	1.48	2.17
$G^{II}_{2,0,0}$	0.17	0.38	0.67	1.00	0.67	1.48	2.59	3.90	0.95	2.09	3.67	5.52	0.67	1.48	2.59	3.90
$G^{II}_{3,0,0}$	0.25	0.56	1.00	1.55	0.98	2.17	3.90	6.01	1.39	3.08	5.52	8.50	0.98	2.17	3.90	6.01
$G^{II}_{0,1,-1}$	0.18	0.40	0.67	0.98	0.48	1.03	1.71	2.49	0.67	1.46	2..42	3.52	0.48	1.03	1.72	2.50
$G^{II}_{1,1,-1}$	0.40	0.88	1.48	2.17	1.03	2.23	3.75	5.51	1.46	3.15	5.31	7.79	1.03	2.24	3.77	5.54
$G^{II}_{2,1,-1}$	0.67	1.48	2.59	3.90	1.71	3.75	6.56	9.87	2.42	5.31	9.28	13.96	1.72	3.77	6.60	9.92
$G^{II}_{3,1,-1}$	0.98	2.17	3.90	6.01	2.49	5.51	9.87	15.20	3.52	7.79	13.96	21.50	2.50	5.54	9.92	15.28
$G^{II}_{0,1,0}$	0.26	0.57	0.95	1.39	0.67	1.46	2.42	3.52	0.96	2.06	3.42	4.99	0.67	1.46	2.42	3.52
$G^{II}_{1,1,0}$	0.57	1.24	2.09	3.08	1.46	3.15	5.31	7.79	2.06	4.47	7.52	11.04	1.46	3.15	5.31	7.79
$G^{II}_{2,1,0}$	0.95	2.09	3.67	5.52	2.42	5.31	9.28	13.96	3.42	7.52	13.14	19.78	2.42	5.31	9.28	13.96
$G^{II}_{3,1,0}$	1.39	3.08	5.52	8.50	3.52	7.79	13.96	21.50	4.99	11.04	19.78	30.45	3.52	7.79	13.96	21.50
$G^{II}_{0,1,1}$	0.18	0.40	0.67	0.98	0.48	1.03	1.72	2.50	0.67	1.46	2.42	3.52	0.48	1.03	1.71	2.49
$G^{II}_{1,1,1}$	0.40	0.88	1.48	2.17	1.03	2.24	3.77	5.54	1.46	3.15	5.31	7.79	1.03	2.23	3.75	5.51
$G^{II}_{2,1,1}$	0.67	1.48	2.59	3.90	1.72	3.77	6.60	9.92	2.42	5.31	9.28	13.96	1.71	3.75	6.56	9.87
$G^{II}_{3,1,1}$	0.98	2.17	3.90	6.01	2.50	5.54	9.92	15.28	3.52	7.79	13.96	21.05	2.49	5.51	9.87	15.20

error bound is not only dependent on the discrepancy of the point grid but also on the norm of the function in the Sobolev space $\mathcal{H}^{\mathrm{II}}_{s,t}(\mathcal{B}_R)$. This, as a consequence gives a dependence on the eigenvalues $A_{m,n}$ and the degree of the orthonormal system $\{G_{m,n,j}\}_{m,n\in\mathbb{N}_0;j=1,2,\ldots,2n+1}$. Hence, the use of an orthonormal system having higher degree will increase the value of error upper bound.

Chapter 8

Conclusions and Outlook

8.1 Summary

The main objective of this work was to develop an equidistribution theory for a 3-dimensional ball together with the construction of the grids on the ball. In particular, our focus was to obtain low-discrepancy point grids. Since such a theory is known for the surface of the ball, it provided the foundation for our work.
We formulated a class of pseudodifferential operators on the ball and used specific Sobolev spaces based on these operators and known orthonormal systems on the ball. These orthonormal systems have their advantages and disadvantages, which were then observed and discussed during the numerical computations. Also, we discussed some properties of these operators. All this theory enabled us then to devise a theory of the discrepancy method for the domain of a ball.
In order to get some nice configurations on the ball, we began with known spherical point grids, i.e. the grids on the surface of the ball. As a first trial, we took these point grids and constructed with them a grid on the ball. At first, we checked the uniformity of these points using their 3-dimensional image on a ball. We also derived a formula, as another quantifying measure, called the generalized discrepancy. This formula depends on the point grids and its value gives us an idea about the equidistribution of the grids on the ball. The point grid with a lower value of discrepancy is considered better than others. With the help of these two techniques, we observed that our initial constructions are not so nicely distributed and have an accumulation of points at the centre of the ball. Aiming to overcome this drawback, we modified these grids by adding an arrangement dependent on the radius. This resulted in better distributions on the ball.

In order to get optimal point grids on the ball, we also tried different algorithms, for example by changing the maximum and minimum distances between the points on the ball or by changing the angles between the points, to find out which of these modifications lead us to an equidistribution criterion. Some of these methods gave good results and faster convergence to a lower value of the discrepancy. Since our focus was to obtain low-discrepancy configurations, this idea led us to another aspect of this problem, which is the implementation of an optimization method, i.e. given a starting grid, we tried to find a grid which minimizes the generalized discrepancy. We used the BFGS optimization technique together with different updates and line search methods for this problem and got some nice grids as a consequence of its application. We observed that the change in the line search or update methods has an effect on the convergence and on the number of iterations. It is evident from the outcomes that the LDL^{T} update in combination with the Wolfe conditions give us the grids with the best discrepancy estimates and for a lower number of iterations in comparison to the other results.
We observed that the generalized discrepancy has some nice statistical and numerical properties. We proved with the help of statistical procedures that the generalized discrepancy actually converges to zero for large enough uniformly distributed grids. This result, indeed, coincides with our numerical results, where the discrepancy estimates decrease with the increase in number of points. We also discovered that the generalized discrepancy is actually the worst case error for our case.
These concepts and numerical results motivated us to generalize the equidistribution theory for the d-dimensional case. For this purpose, we first formulated orthonormal systems for dimension d and then constructed the function spaces and differential operators based on them. Moreover, we derived the discrepancy formula and did some tests for the case $d = 4$. These results showed that the techniques we constructed for the 3-dimensional case work also well for the higher dimensions. Since a common problem that we encounter in higher dimensions is the increase of cost, we also discussed the tractability of integration in our Sobolev spaces and found out the conditions under which the integration is tractable in our settings.
We also tested our grids using some examples for the numerical integration on the ball. Although these results can prove to be a good starting point for such experiments on the ball, there is room for further research and improvements in this regard.

8.2 Outlook for Future Investigations

This work raises some new questions and opens the route for further investigations.
We formulated the theory of equidistribution for the domain of a ball but were restricted to some cases. For example, the choice of function spaces and the differential operators is confined. We worked with Sobolev spaces that are dependent on a specific class of pseudodifferential operators. Thus, further experiments can be done in this regard, as a different class of operators may improve the estimates. Moreover, the BFGS method examined in Chapter 4, can also be considered for higher degrees of the orthonormal basis systems, i.e. by truncating the sum in the discrepancy formulae and their gradients for larger degrees m and n. Also, further tests with the BFGS method can be done by considering the grids with the weighted discrepancies. From the results for the numerical integration on the ball (Chapter 7), we assume that the specific pseudodifferential operator we used and, consequently, its eigenvalues affect the results. This opens up the question for finding a different operator or the construction of a new Sobolev space which can improve the results.
Further, other equidistributed spherical grids, for example the spiral grid ([25]), can also be considered for the construction of the grids on the ball. A further concept that needs to be investigated is: a quadrature-independent approach in order to find a tool as another quantifying measure of the points. This approach will be helpful in the sense that it will not be dependent on the differential operators.
Another question of interest is: how can one extend this theory of equidistribution to the subdomains of a ball. If we want to observe how well the grid points are distributed on an arbitrary subdomain of a ball, we require an analysis theory that works particularly for this case. This can be investigated, for example, by using an ansatz motivated by the spherical approach in [21, 35] .
The implementation of the theory of this thesis and the constructed grids to a real problem, for example, in the algorithms like RFMP and ROFMP or to the regularization and approximation problems is also a future work. The implementation of this theory to the inverse MEG/EEG problems is realized in [42].

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