Mathematisches Institut

Justus-Liebig-Universität Giessen

Advances in radial and spherical basis function interpolation

Dissertation

zur Erlangung des Doktorgrades
der Naturwissenschaftlichen Fachbereiche der
Justus-Liebig-Universität Gießen

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14 December 2018

Abstract:

The radial basis function method is a widely used technique for interpolation of scattered data. The method is meshfree, easy to implement independently of the number of dimensions, and for certain types of basis functions it provides spectral accuracy. All these properties also apply to the spherical basis function method, but the class of applicable basis functions, positive definite functions on the sphere, is not as well studied and understood as the radial basis functions for the Euclidean space. The aim of this thesis is mainly to introduce new techniques for construction of Euclidean basis functions and to establish new criteria for positive definiteness of functions on spheres.

We study multiply and completely monotone functions, which are important for radial basis function interpolation because their monotonicity properties are in some cases necessary and in some cases sufficient for the positive definiteness of a function. We enhance many results which were originally stated for completely monotone functions to the bigger class of multiply monotone functions and use those to derive new radial basis functions. Further, we study the connection of monotonicity properties and positive definiteness of spherical basis functions. In the processes several new sufficient and some new necessary conditions for positive definiteness of spherical radial functions are proven.

We also describe different techniques of constructing new radial and spherical basis functions, for example shifts. For the shifted versions in the Euclidean space we prove conditions for positive definiteness, compute their Fourier transform and give integral representations. Furthermore, we prove that the cosine transforms of multiply monotone functions are positive definite under some mild extra conditions. Additionally, a new class of radial basis functions which is derived as the Fourier transforms of the generalised Gaussian $\phi(t) = e^{-t^\beta}$ is investigated.

We conclude with a comparison of the spherical basis functions, which we derived in this thesis and those spherical basis functions well known. For this numerical test a set of test functions as well as recordings of electroencephalographic data are used to evaluate the performance of the different basis functions.

'I have learnt that all our theories are not Truth itself, but resting places or stages on the way to the conquest of Truth, and that we must be contented to have obtained for the strivers after Truth such a resting place which, if it is on a mountain, permits us to view the provinces already won and those still to be conquered.'

— Justus von Liebig
(Liebig to Gilbert 1870)

Acknowledgement:

First, I wish to thank my advisor, Prof. Martin Buhmann for the guidance and kind support he offered ever since I was a Bachelor student. His enthusiasm and his insight for mathematics in general and for approximation theory in specific were an inspiration. Despite his many commitments in the university and the Mathematikum, he always took time to discuss my research, problems as well as successes. He gave me the opportunity to present my findings at international conferences and never ceased to show that math, in fact, makes you happy.

I extend my thanks to Prof. Oleg Davydov of the numerical analysis group for interesting lectures and our constructive cooperation on various courses. Furthermore I would like to thank my colleagues for making the four years of my Ph.D. a pleasant and educational experience.

Besonderer Dank gebührt den wunderbaren Menschen meiner Familie für ihre fortwährende Unterstützung. Vor allem danke ich meinem Freund, Michael Wagner, der mich während der Entstehung dieser Arbeit mit einem Höchstmaß an Verständnis begleitet hat.

Contents

Outline

Interpolation of scattered data using radial basis functions is a widely used technique with various applications. The method was originally developed for interpolation in Euclidean spaces but has been adapted for interpolation of scattered data on spheres and other manifolds. The interpolation problem which is addressed by the radial or spherical basis function method has the form:

Given a set of centres $\Xi \subset A$ and a set of corresponding values $f(\xi)$, $\xi \in \Xi$, find a function $s : A \to \mathbb{R}$ satisfying

$$s(\xi) = f(\xi), \quad \xi \in \Xi.$$

In the first three chapters A will be the Euclidean space $\mathbb{R}^d$ and in the fourth chapter we will focus on $A = \mathbb{S}^{d-1}$. The interpolants will be formed from linear combinations of shifts of radial basis functions or spherical basis functions. We start in the first section by giving an introduction to scattered data interpolation in the Euclidean space and to the theory of radial basis function interpolation.

In the second chapter we study multiply and completely monotone functions. Those are functions, which satisfy certain conditions on the signs of their derivatives. The functions are important because the monotonicity properties are in some cases necessary and in some cases sufficient for the positive definiteness of a basis function. We sum up existing results on their properties and enhance many of them, where possible. The theorems we extend are Theorems 2.9 to 2.16. Theorem 2.20 and Theorem 2.21 are new results on multiply monotone functions. We then derive, from the aforementioned results, examples of new radial basis functions (see Example 2.22).

We start the third chapter by proving that the cosine transforms of multiply monotone functions are positive definite under some mild extra conditions (Theorem 3.1 and Theorem 3.5). To our knowledge this connection has not been described before. We then, in Section 3.2, study shifts of radial basis functions and give a formula to compute the multivariate Fourier transform of such shifts (Theorem 3.14). We also provide further results on the positive definiteness and representation of such shifted basis functions (Theorem 3.8-Lemma 3.12). In Section 3.3 we introduce a new class of radial basis functions which is derived as the Fourier transforms of the generalised Gaussian $\phi(t) = e^{-t^\beta}$. This section was inspired by a paper by Boyd and McCauley [BM13] who introduced the inverse quartic Gaussian as the 1-dimensional Fourier transform of $\phi(t) = e^{-t^4}$. We are interested in the d-dimensional Fourier transforms of $\phi(t) = e^{-t^\beta}$, since this class of functions includes the Poisson as well as the Gaussian kernel. In Theorem 3.23 we give a series representation for this class of positive definite basis functions for the case $\beta > 1$.

In the fourth chapter of this thesis we study interpolation on spheres a topic which received increasing attention during the last years. After we introduce the necessary definitions and results in the first section. We, in Section 4.2, state new criteria for the positive definiteness of such spherical basis functions. Two of the most important new results are presented in Theorem 4.23 and Theorem 4.27. The importance of monotonicity properties for positive definite spherical functions is one of the key results of this thesis. We sum up our findings on the sufficient (and sometimes necessary) conditions of monotonicity for spherical basis functions in Section 4.2.1. In the remainder of Chapter 4 we study a shifted version of the surface spline for the sphere, compute its Fourier coefficients in Theorem 4.41 and so deduce their decay properties. These decay properties are important to determine error estimates of the interpolation. We additionally point out two observations on shifts as well as scaling of basis functions for the sphere in Theorem 4.43 and Lemma 4.45.

In the final chapter of this thesis we perform numerical tests on the spherical basis functions derived from Chapter 4 and compare their performance to some well known basis functions as the Gaussian and the inverse multiquadric. We thereafter use the methods which performed best to reconstruct data which was recorded by an electroencephalogram.

Chapter 1

Introduction

In this thesis we mainly focus on the topic of data interpolation. Interpolation of data which were found by sampling a function, is a problem that occurs in various fields, like engineering, physics, geoscience and medicine. Many of these applications require to fit a function f which is given on $\mathbb{R}^2$, $\mathbb{R}^3$, or higher dimensional Euclidean spaces. In applications, the function which is sampled is often unknown outside the sample set, this is for example the case for temperature measurements in the ocean or the heights of a mountain range. Or it is to computationally expensive to evaluate the function, a problem common in physics, then the goal is to find an approximating function which can be easily evaluated.

Values of the function will be known in a finite set of distinct points $\Xi \subset \mathbb{R}^d$. The goal is to find an approximant $s : \mathbb{R}^d \to \mathbb{R}$ which satisfies the interpolation condition

$$s(\xi) = f(\xi),$$

for all $\xi \in \Xi$.

As the examples suggest the data sites will seldom be given on a d-dimensional grid ($\Xi \subset h\mathbb{Z}^d$, $h \in \mathbb{R}_{>0}$) but will be scattered in $\mathbb{R}^d$. Also the distribution of the data sites might be predetermined and therefore cannot be chosen to fit requirements of the approximation technique. We will in the remainder of this section present some approximation techniques, like polynomial interpolation, which pose such requirements on the distribution of the data sites. One example of a situation where the distribution of sites can not be changed, is described in [JKBS16], where the interpolation of electroencephalographic (EEG) data is examined. There are several standard distributions of electrodes used to measure the EEG, the so called 10/20 system with 19 electrodes is most common but there are also measurements with 32 or 64 electrodes. Those distributions are used in nearly all clinical EEG measurements, so changing these distribution is not an option. Therefore the method used has to be applicable to the given distribution of data sites.

The adaptability to such data sets is an important reason why there is a need for interpolation techniques that provide solutions of the interpolation problem for arbitrary data number and distribution. In the one dimensional case there are various techniques available which meet this requirement. Examples are polynomial and spline interpolation.

For higher dimensions many of those techniques fail the solvability requirement. This is because we know that for any finite set of (data independent) basis functions,

$$\phi_1, \ldots, \phi_n : \mathbb{R}^d \to \mathbb{R},$$

we can choose a set of distinct data sites $\Xi \subset \mathbb{R}^d$, so that the interpolation problem $s(\xi) = f(\xi),\ \forall \xi \in \Xi$, has no solution of the form

$$s(x) = \sum_{i=1}^{n} a_i \phi_i(x), \quad a_i \in \mathbb{R},\ i = 1, \ldots n.$$

The statement is known as Mairhuber-argument and was first proven in [Mai56].

1.1 Methods for approximation in Euclidean spaces

Before we start with the description of the radial basis function method we give a short introduction to some other methods for multivariate interpolation of scattered data. Because we want to investigate a multivariate interpolation problem, the following multi-index notation will be frequently used:

Definition 1.1. *For $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{Z}^n_{\geq 0}$ and $\beta \in \mathbb{Z}^n_{\geq 0}$ we define*

$$\begin{aligned}
&\alpha! = \alpha_1! \cdot \cdots \cdot \alpha_n!,\\
&\alpha - \beta = (\alpha_1 - \beta_1, \ldots, \alpha_n - \beta_n),\\
&x^\alpha = x_1^{\alpha_1} \cdot \cdots \cdot x_n^{\alpha_n},\\
&\beta \leq \alpha \textit{ if and only if } \alpha - \beta \in \mathbb{Z}^n_{\geq 0},\\
&D^\alpha = D_1^{\alpha_1} \cdot \cdots \cdot D_n^{\alpha_n}.
\end{aligned}$$

The examples we give of the techniques are of course not exhaustive, there are various techniques available and we only give introductions to three of them. Also our goal is to describe the ideas of the techniques and their connections to radial basis functions with as little definitions as necessary.

1.1.1 Polynomial interpolation

As stated in the introduction, finding an interpolant to a finite set of distinct data sites $\Xi \subset \mathbb{R}^d$ of the form

$$s(x) = \sum_{j=1}^{N_{d,m}} c_j p_j(x), \quad x \in \mathbb{R}^d,$$

where $\{p_j \mid j = 1, \ldots N_{d,m}\}$ forms a basis of the polynomial space $\mathbb{P}^d_m$ and $N_{d,m} = \dim(\mathbb{P}^d_m)$, is not possible for all sets Ξ. The problem is nevertheless uniquely solvable if the matrix $\{p_j(\xi)\}_{j=1\ldots N_{d,m},\ \xi\in\Xi}$ is non-singular. Sets Ξ with this property are called unisolvent with respect to the function space $\mathbb{P}^d_m$. We define this property in a general form for later use.

Definition 1.2. *A set $X \subset \mathbb{R}^d$ is called* unisolvent *with respect to a functions space W if every element $w \in W$ is uniquely determined by its values in X.*

The construction of those unisolvent sets as well as finding sets with desirable property (as for example error minimisation) are topics of ongoing research in multivariate polynomial interpolation. We describe two cases where multivariate polynomial interpolation is possible for special sets of data sites and then briefly introduce a technique which allows interpolation of arbitrary sets.

The first one uses tensor product polynomials for interpolation of data, which is given on a multivariate grid. The space of tensor product polynomials is defined as

$$\overline{\mathbb{P}}_k^d = \left\{ \sum_{\alpha \le k} c_\alpha x^\alpha \middle| c_\alpha \in \mathbb{R} \right\},$$

where $k \in \mathbb{Z}_{\ge 0}^d$. Each tensor product polynomial has a unique representation as tensor product of the univariate polynomials because

$$\overline{\mathbb{P}}_k^d = \bigotimes_{i=1}^d \overline{\mathbb{P}}_{k_i}^1,$$

with $\dim\left(\overline{\mathbb{P}}_k^d\right) = (k_1 + 1) \cdot (k_2 + 1) \cdots (k_d + 1)$.

A suitable set for interpolation using tensor product polynomials is any tensor product grid $\Xi \subset \mathbb{R}^d$, which means $\Xi = \bigotimes_{i=1}^d \Xi_i$, where $\Xi_i \subset \mathbb{R}$ is a set of distinct points in $\mathbb{R}$. So each element $\xi \in \Xi$ has the form $\xi = (\xi_1, \ldots, \xi_d)^T$ where $\xi_i \in \Xi_i$.

An interpolating function $s \in \overline{\mathbb{P}}_k^d$ can be written as a product of univariate Lagrange-polynomials. Let $L_{\xi_i}^i(x_i)$ be the univariate Lagrange interpolation polynomial to the element $\xi_i \in \Xi_i$, meaning $L_{\xi_i}^i(\xi_i) = 1$ and $L_{\xi_i}^i(\zeta) = 0$ for all $\zeta \in \Xi_i \setminus \{\xi_i\}$. Then the solution to the above interpolation problem can be given as

$$s(x) = s\left((x_1, \ldots, x_d)^T\right) = \sum_{\xi \in \Xi} f(\xi) \prod_{i=1}^d L_{\xi_i}^i(x_i).$$

One advantage of this method is that error estimates of the interpolation can be derived easily using the estimates known from univariate polynomial interpolation. One obvious drawback is the need of the data to be given on a tensor product grid.

A second type of data distribution allows the interpolation using polynomials of total degree. The unisolvent sets are in this case constructed using a simplex grid. For a set of distinct points $t_1, \ldots, t_{d+1} \in \mathbb{R}^d$ which are not part of one hyperplane, we define the simplex

$$S = \left\{ \sum_{i=1}^{d+1} c_i t_i \middle| c_i \in \mathbb{R}_{\ge 0}, \sum_{i=1}^{d+1} c_i = 1 \right\}.$$

The simplex grid is now defined as

$$D_{n,S} = \left\{ \xi_\alpha = \frac{1}{n} \sum_{i=1}^{d+1} \alpha_i t_i \middle| \alpha \in \mathbb{Z}_{\geq 0}^{d+1},\ |\alpha| = n \right\}.$$

In this case $|D_{n,S}| = \binom{n+d}{d} = N_{d,m}$ and $D_{n,S}$ is a unisolvent set for $\mathbb{P}_n^d$. For these point sets error estimates can be derived using Lebesgue functions and the Lebesgue constant. For example de Marchi et al. [BCM+06] studied how point sets can be created which minimise these functions and thereby have optimal error estimates.

The obvious polynomial reproducing properties of these interpolants are one of the strengths of this technique. Still one can not perform a polynomials interpolation if the given set of data sites is not a unisolvent set. To overcome this problem one can use higher degree polynomials. Several techniques allow us to find an interpolant $s \in \mathbb{P}_d^{m-1-\nu}$ to a set of data sites $\Xi \subset \mathbb{R}^d$ with $|\Xi| = m$. Some examples are the Hakopian interpolation described in [Hak82] and the technique described by Kergin [Ker80]. In the case of the Kergin interpolation it was proven that if the target function is m-times continuously differentiable and $\Xi \subset \mathbb{R}^d$ consists of $m+1$ not necessarily distinct points, then there exists a polynomials of total degree at most m which interpolates f in Ξ. If a point appears in Ξ ℓ-times then the derivative of f is interpolated in this point up to the $(\ell - 1)-$st derivative. The existence of this interpolating polynomial was proven by P. Kergin in 1980 and in the same year C. Micchelli and P. Milman established a formula for its computation in [MM80].

For a more comprehensive description of the existing multivariate polynomial interpolation techniques we recommend the paper [GS00] by Gasca and Sauer. In most of the described methods the degree of the polynomials used for interpolation grows with the number of data sites which can lead to unwanted oscillation of the interpolant. Also interpolants will always satisfy $|s(x)| \to \pm\infty$ for $\|x\| \to \infty$ if the degree of the polynomial is not zero. The introduction of spline basis functions allows to overcome these two problems.

1.1.2 Spline interpolants

Spline interpolants and quasi-interpolants were studied intensively for the last 50 years and they are widely used for the approximation of functions. Splines as piecewise polynomials have many desirable properties. They are very easy to evaluate and it is also straightforward to compute their derivatives or integrals. Mainly, they combine the advantages of polynomials which are very simple when regarded in a local context, with an extreme flexibility on a larger scale. Also the approximation orders are known exactly, if the smoothness property of the function to be approximated is suitable.

Splines were developed in one dimension first and then different generalisations to multivariate settings were described. The basic definitions about splines are briefly recaptured before we describe the multivariate interpolation techniques.

Let us introduce a strictly monotonically increasing finite sequence of knots $\triangle := \{x_i\}_{i=0}^{n}$ with $a = x_0 < \cdots < x_n = b$. Also let $\nu := \{\nu_i\}_{i=0}^{n}$ be a sequence corresponding to $\triangle$ which describes the smoothness conditions that the spline should satisfy at the points x_i, meaning that the spline should be $\nu_i - 1$ times continuously differentiable at the knot x_i. The Schoenberg space of splines of order k, corresponding to the sequences $\triangle$ and ν, is defined by

$$S_k(\triangle, \nu, A) = \left\{ s : A \to \mathbb{R} \mid s|_{[x_i, x_{i+1}]} \in \mathbb{P}_{k-1} \textit{ and } s \in C^{\nu_i - 1} \textit{ at } x_i \right\},$$

with $A = [a, b] \subset \mathbb{R}$.

The most common choice is $\nu = (k-1, \ldots, k-1)$, where all elements of the space have smoothness $k-1$ on $[a, b]$. The dimension of this space for a finite knot sequence with $n+2$ distinct knots is $n+k$.

To define the common B-spline basis, we combine the two sequences mentioned earlier so we will only need one sequence for the definition of the basis. The new sequence allows the repetition of a value and the value x_i appears in this series $k - \nu_i$ times. So each repetition means that one order of smoothness is lost. We denote this new series by $T = \{t_i\}_{i=-k+1}^{m+k}$ for $A = [a, b]$ where we set $t_{-k+1} = \cdots = t_0$ and $t_m = t_{m+1} = \cdots = t_{m+k-1}$ and identify $S_k(\triangle, \nu, A) = S_k(T, A)$ as two ways of describing the same space. One special spline is the truncated power function

$$(x)_+^{\ell} := \begin{cases} x^{\ell}, & \text{for } x > 0, \\ 0, & \text{if } x \leq 0, \end{cases} \qquad \ell \in \mathbb{N}.$$

This spline is used to describe a basis of the spline space. We will also use it throughout this thesis because it is important for the class of multiply monotone functions. The normalized B-spline is now defined using the divided differences as

$$N_{i,k,T}(x) = (t_{i+k} - t_i)[t_i, \ldots, t_{i+k}](\cdot - x)_+^{k-1}.$$

We call $N_{i,k,T}$ the i-th B-Spline of order k to the knot sequence T. These B-splines have important properties, i.e. for given k, T and A, that

1. $N_i(x) \geq 0$ for all $x \in A$,

2. $\operatorname{supp} N_i \subset [t_i, t_{i+k}]$,

3. $\sum_{i=-k+1}^{m+k} N_i(x) \equiv 1$ for all $x \in A$.

For more information on the definition and the basic properties of the B-splines we recommend the introductory books of de Boor [dB90], [dB01], for a collection of theoretical results on approximation power see the work of DeVore, [DL93], and for modelling and computational methods see [HH13] and [Sch15]. Before we use splines for multivariate interpolation we make a few remarks about interpolation using splines. One problem not occurring in radial basis function interpolation is that for a given finite set of data sites $\Xi \subset A$ and corresponding function values $\{f(\xi)\}_{\xi\in\Xi}$, to find a unique spline interpolant, the dimension of the spline space has to be equal to the number of data sites $|\Xi| = n$. Choosing a set of spline basis functions according to a given data set is therefore not as easy as it is for radial basis functions, especially when multivariate approximation is needed as will be described. For very low order spline spaces there are exceptions to this problem. When for example the interpolants are to be chosen from the space of linear functions, the knot series T can be defined using the data sites $\Xi = \{\xi_1, \ldots, \xi_n\}$, which satisfy $\xi_i < \xi_{i+1}$. Setting $t_i = \xi_{i+2}$ for $i = -1, \ldots n-2$ an interpolant can be given by

$$s(x) = \sum_{i=1}^{n} f(\xi_i) N_{i-2,2,T}(x), \quad x \in \mathbb{R}.$$

We mention here that this interpolant is the same one we will find as a univariate radial basis function interpolant when choosing our basis function to be the linear, $\phi(r) = r$, as will be explained later. This simple interpolation operator can only be stated in this form because the B-splines of order 2 form a basis of Lagrange functions, whereas if we want to find an interpolant of higher order we usually have to choose the spline space according to the data sites in a more elaborate way or check if the data sites satisfy conditions as the Schoenberg-Whitney conditions.

Theorem 1.3 (Schoenberg-Whitney)**.** *Let $\Xi \subset A$ be a set of $n+k$ distinct data site with $\xi_i < \xi_{i+1}$. The interpolation problem*

$$s(\xi) = f(\xi), \quad \forall \xi \in \Xi,$$

has a unique solution $s \in S_k(\triangle, k-1, A)$ *if and only if*

$$\xi_i < x_i < \xi_{i+k}, \quad i = 1, \dots, n-1.$$

If this condition holds there are interpolating operators and good error estimates available. Also it is easy to prove that in this setting the interpolant satisfies

$$s(x) \equiv f(x), \quad \forall x \in A,$$

for all $f \in \mathbb{P}_{k-1}$.

For the multivariate setting there are several possible ways of generalisation. We start with the more straightforward approach of tensor product B-Splines which uses tensor products of univariate splines. The results from univariate interpolation extend immediately to this setting, but it is only applicable to gridded knots. Moreover, the piecewise polynomial degrees are only limited with respect to each variable (component-wise) which is less desirable than to limit the total degree. Nonetheless, we start by stating the theory of tensor product splines before introducing how one can perform interpolation on a triangulation of a given domain. The construction of the interpolating operators is quite similar to the polynomial interpolation only one has to choose a knot sequence defining the B-splines of the desired order which allows to form Lagrange interpolants for the sets Ξ_i in each dimension. Tensor product splines are defined using a tensor product grid. For every coordinate t_ℓ, $\ell = 1, \dots, d$, in $\mathbb{R}^d$, we use one r_ℓ-extended sequence defined as follows;

$$T_\ell = \{t_{j_\ell,\ell}\}_{j_\ell=1}^{n_\ell} \text{ with } t_{j_\ell,\ell} \leq t_{j_\ell+1,\ell} \text{ and } t_{j_\ell,\ell} < t_{j_\ell+r_\ell,\ell},$$

and define the tensor product grid

$$T = T_1 \otimes \cdots \otimes T_d.$$

For every $j \in \mathbb{Z}^d_{>0}$ with $j \leq (n_1, \dots n_d)$ there is one element $\bar{t}_j = (t_{j_1,1}, \dots, t_{j_d,d})$ in T.

Definition 1.4. *The d-variate B-Spline of order* $k = (k_1, \dots, k_n)$ *with respect to the knot series* T *is defined by*

$$N_{k,j}\left((t_1, \dots, t_d)^T\right) = \prod_{\ell=1}^{d} N_{k_\ell, j_\ell, T_\ell}(t_\ell).$$

Most of the properties of the univariate B-Spline apply component-wise to these multivariate B-Splines. The interpolation operators for tensor product splines are derived from univariate interpolants exactly the same way they were for multivariate polynomials, as products of univariate Lagrange interpolants. This means that interpolation to a set $\Xi \subset \mathbb{R}$ of data sites is only possible if Ξ is a tensor product grid and the univariate sequences Ξ_ℓ and T_ℓ satisfy the Schoenberg-Whitney condition. If this is the case, error estimates are easily derived by making use of the univariate polynomial reproducing properties of the B-Splines.

We described for the univariate case how the knot sequence can be chosen in a way allowing the interpolation of a given set of data points. For the multivariate setting this is also possible for low order splines in low dimensions. The process becomes increasingly difficult in higher dimensions. We focus therefore on the case of approximation in two dimensions. The problem there can be solved by defining splines on a triangulation of the area to be approximated. A triangulation is given if the area Ω is decomposed into triangles $\mathcal{T}_1, \ldots, \mathcal{T}_n$ which satisfy $\cup_{i=1}^{n} \mathcal{T}_i = \overline{\Omega}$ and the triangles intersect at most in one corner or one edge.

The spline space for this triangulation is then the space of functions which are polynomials when restricted to one triangle and which satisfy smoothness conditions in the edges and vertices. The construction of interpolants from this spline space is not simple in a general setting. A paper including the construction of triangulations as well as the construction of admissible point sets for interpolation is [DNZ99] by Davydov et al. Even determining the dimension of the spline space is not trivial, but there are special cases in which interpolation can be derived easily. We give a basic example:

If the distribution of the data sites allows to choose a subsets of the sites to be the vertices of the triangulation while each of the remaining data sites is situated on one edge. Meaning there is exactly one data site on each edge and one in each vertex. Then values in these points can be interpolated using a quadratic spline which is continuous in the edges and corners.

Usually it is not easy to find such triangulations for a given set of scattered data. One option is to choose the data sites as corners of the triangulation and then add additional information on the vertices using other approximation techniques.

Splines also allow the construction of quasi-interpolants and Hermite interpolants dependent on the derivatives or integrals of the function to be approximated. For the multivariate setting Box-splines have proven to be a very useful tool because being piecewise polynomials allows to easily achieve polynomial reproduction, even without the interpolation condition. For further information on the topic of spline quasi-interpolation we refer the reader to the work of de Boor [dB01].

Nevertheless for scattered data interpolation in a multivariate setting these techniques are not easily implementable and neither are they easily adaptable to changing data distribution. In contrast to the radial basis function method or the moving least squares method, which we describe in the next section.

1.1.3 Moving least squares

For the moving least squares method we for now drop the interpolation condition and solve a minimisation problem instead. The approximant $s : \mathbb{R}^d \to \mathbb{R}$ to a function f for which we know a set of function values $f(\xi)$, $\xi \in \Xi$, satisfies: $s(x) = p^*(x)$ where $p^* \in \mathbb{P}_m^d$ is the solution of

$$\operatorname{argmin}\left\{\sum_{\xi\in\Xi}\left(f(\xi)-p(\xi)\right)^2 w(x,\xi) :\ p\in\mathbb{P}_m^d\right\}.$$

The weight function $w : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is usually decaying with the Euclidean distance between its arguments or is even compactly supported.

The approach is especially useful if only finitely many evaluations of the approximant are needed, also the size of the problem can be adjusted by changing the weight function.

Often radial basis functions are used as weight functions but also multivariate splines are possible choices. It can be proven that this approximant under some conditions on the weight function reproduces polynomials of order $\mathbb{P}_m^d$ also the problem is equivalent to the following version:

$$\min\left\{\frac{1}{2}\sum_{\xi\in I}\Psi_\xi(x)^2\frac{1}{w(x,\xi)}\right\}$$

under the condition that

$$\sum_{\xi\in I}\Psi_\xi(x)p(\xi) = p(x), \quad \forall p\in\mathbb{P}_m^d,$$

where I is the subset of Ξ with $w(x,\xi)\neq 0$. The approximant then has the form

$$s(x) = \sum_{\xi\in I} f(\xi)\Psi_\xi(x).$$

This version is called the Backus-Gilbert approach.

The case of $m = 0$ is known as Shepard's method. The approximant in this case has the form

$$s(x) = \frac{\sum_{\xi \in I} f(\xi) w(x, \xi)}{\sum_{\xi \in I} w(x, \xi)}.$$

A traditional choice of the weight function is in this case a power of an inverse distance $w(x, \xi) = \frac{1}{\|x-\xi\|^p}$. The method is then referred to as inverse distance weighting. Because of the form of the approximant interpolation is achieved but the approximant has a zero derivative in the data sites if $p \geq 1$. This is one disadvantage of the technique in this form.

The approximation power of the moving least squares method was studied for example by D. Levin in [Lev98]. Lately various methods combining moving least squares and radial basis functions were suggested and give highly accurate results, see for example [Fas07] and [Wen05]. We now turn to the definition of this radial basis function technique which is the core of this thesis.

1.2 Radial basis functions in Euclidean spaces

We start by defining radial basis functions.

Definition 1.5. *A radial basis function is a function* $\Phi : \mathbb{R}^d \to \mathbb{R}$*, which is radially symmetric, s.t.:* $\Phi(x) = \Phi(y),\ \forall x, y \in \mathbb{R}^d$ *satisfying* $\|x\|_2 = \|y\|_2$.

A radial basis function Φ can therefore be derived from a one-dimensional function $\phi : \mathbb{R}_{\geq 0} \to \mathbb{R}$, in a way that $\Phi(x) = \phi(\|x\|_2)$ holds for all $x \in \mathbb{R}^d$. We refer to Φ and ϕ both as a radial basis function. Since we mostly use the Euclidean norm throughout the next chapters we denote it with $\|\cdot\|$ for simplicity. If a different norm is referred to it will be specifically declared. Some examples of well known and studied radial basis functions are:

- The **multiquadrics** which were first described in [Har90] by Hardy. The good properties they have, when used for interpolation, were studied, for example, in [Fra82] and [Buh03]. The generalised multiquadric basis function is given by

$$\phi(r) = (r^2 + c^2)^\beta, \quad c > 0, \quad 0 < \beta \notin \mathbb{N},$$

  where c is a shape parameter. The classical form of the multiquadric is derived by choosing $\beta = 1/2$. By choosing $\beta < 0$ the class called the inverse multiquadrics can be derived.

- The widely used **Gaussian** basis function

$$\phi(r) = e^{-\alpha r^2}, \quad \alpha > 0.$$

- The **Wendland functions** (see [Wen96] and Appendix A) which are the first of the mentioned radial basis functions to have compact support. The functions are derived from a one-dimensional polynomial $p(r)$ by

$$\phi(r) = \begin{cases} p(r), & \text{for } 0 \leq r \leq 1, \\ 0, & \text{otherwise.} \end{cases}$$

  The polynomial has to be chosen according to the dimension of the space and the smoothness required. One example in $\mathbb{R}^3$ is $\phi(r) = (1-r)_+^8(32r^3 + 25r^2 + 8r + 1)$.

- The **Matérn** radial basis function described in [MB02] is given by:

$$\phi(r) = r^{\nu} K_{\nu}(r), \quad \nu > 0,$$

where K_{ν} denotes the modified Bessel function ([AS72], 9.6.25) with the integral representation:

$$K_{\nu}(xz)x^{\nu} = \frac{\Gamma(\tau + \frac{1}{2})(2z)^{\nu}}{\pi^{\frac{1}{2}}} \int_0^{\infty} \frac{\cos(xt)}{(t^2 + z^2)^{\nu + \frac{1}{2}}}\, dt, \tag{1.1}$$

when $\mathcal{R}\tau > -\frac{1}{2}$, $x > 0$, and $|\arg z| < \frac{1}{2}\pi$.

1.3 Interpolation using radial basis functions

We focus, for the first part of this thesis, on solving multivariate interpolation problems of the following form.

Problem 1.6. *Given a set of centres $\Xi \subset \mathbb{R}^d$, and a set of function values $f(\xi)$, for all $\xi \in \Xi$, stemming from a possibly unknown target function $f : \mathbb{R}^d \to \mathbb{R}$. An interpolant $s : \mathbb{R}^d \to \mathbb{R}$, is to be computed satisfying*

$$s(\xi) = f(\xi), \quad \forall \xi \in \Xi. \tag{1.2}$$

There are many ways to construct multivariate interpolants, some were described in Section 1.1, but for radial basis function interpolation we will form the approximant as a linear combination of shifts of one radial basis function, so that the centres of the basis functions lie in the data sites. Therefore the interpolant has the form:

$$s(x) = \sum_{\xi \in \Xi} c_\xi \phi(\|x - \xi\|), \quad x \in \mathbb{R}^d, \tag{1.3}$$

where $c_\xi \in \mathbb{R}$ are chosen so that (1.2) holds if possible. The coefficients $c_\xi \in \mathbb{R}$ are computed by solving the set of linear equations:

$$f = A_\Xi c, \tag{1.4}$$

where $f = \{f(\xi)\}_{\xi \in \Xi}$, $c = \{c_\xi\}_{\xi \in \Xi}$, and

$$A_\Xi = \{\phi(\|\xi - \zeta\|)\}_{\xi, \zeta \in \Xi}.$$

The matrix A_Ξ will be referred to, in what follows, as the interpolation matrix.

1.3.1 Solvability of the interpolation problem

We know now that computing the solution of the system of linear equations is equivalent to the computation of the interpolant and therefore the unique solvability is formally given if the interpolation matrix is nonsingular. One important criterion for the non singularity of a symmetric matrix is positive definiteness. The matrix A is positive definite if

$$c^T A c > 0, \quad \forall c \in \mathbb{R}^n \setminus \{0\}. \tag{1.5}$$

The interpolation matrix of ϕ, A_Ξ, is of course symmetric. A positive definite interpolation matrix thereby means that the interpolation problem is solvable.

Definition 1.7. *A function $\Phi \in C(\mathbb{R}^d)$ is called* conditionally strictly positive definite of order m, *$m \in \mathbb{N}$ (c.s.p.d.(m)) on $\mathbb{R}^d$, if for any finite set of distinct points $\Xi \subset \mathbb{R}^d$, the matrix $A_\Xi = \{\Phi(\xi - \zeta)\}_{\xi,\zeta \in \Xi}$, is positive definite on the subspace*

$$\mathbb{P}^d_{m-1}|^{\perp}_{\Xi} = \left\{ c \in \mathbb{R}^{|\Xi|} \middle| \sum_{\xi \in \Xi} c_\xi p(\xi) = 0, \forall p \in \mathbb{P}^d_{m-1} \right\}. \tag{1.6}$$

If for any finite set of distinct points $\Xi \subset \mathbb{R}^d$, the matrix A_Ξ, is positive definite on $\mathbb{R}^d$, the function is called strictly positive definite,*(s.p.d.) on $\mathbb{R}^d$.*

This property is not only applicable to radial functions, so the class we call *c.s.p.d.*(m) includes more than just radial functions. When using a strictly positive definite function to solve the interpolation problem (1.2), there is always a unique solution of the form (1.3). When using a function only conditionally strictly positive definite of a given order m, solvability can be obtained by adding low order polynomials. The interpolant is then of the form

$$s(x) = \sum_{\xi \in \Xi} c_\xi \phi(\|x - \xi\|) + p(x), \tag{1.7}$$

where $p \in \mathbb{P}^d_{m-1}$, is a polynomial of total degree $m - 1$. This interpolation problem can be rewritten as

$$\begin{pmatrix} A_\Xi & P \\ P^T & 0 \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix} \text{ mit } P = (p_k(\xi))_{\xi \in \Xi, k \in \{1,\dots,j\}}, \tag{1.8}$$

where the polynomials $p_k \in \mathbb{P}^d_{m-1}$ form a basis of the polynomial space $\mathbb{P}^d_{m-1}$ and $j = \dim(\mathbb{P}^d_{m-1})$. To obtain unique solvability we have to use the property of unisolvency defined in Definition 1.2.

Theorem 1.8. *For $\Phi \in C(\mathbb{R}^d)$ being a conditionally strictly positive definite function of order m, the interpolation problem* (1.2) *is solvable with a unique solution of the form* (1.7) *if and only if Ξ has a unisolvent subset with respect to $\mathbb{P}^d_{m-1}$.*

The property of strict positive definiteness of a certain function can not be derived easily from the above definition. Therefore there have been several approaches to characterise positive definite functions (see, for example [SW01]). We start by introducing a new concept which is fundamental for the rest of this thesis and which will be discussed and used, in a generalised form, in Chapter 2 and Section 4.2.

Definition 1.9. *A function $g : \mathbb{R}_{>0} \to \mathbb{R}$ is called* completely monotone of order m *if and only if it is in $C^\infty(\mathbb{R}_{>0})$ and*

$$(-1)^\ell g^{(\ell)}(t) \geq 0, \quad \forall t > 0, \tag{1.9}$$

holds for all $\ell \geq m$. Being completely monotone of order m implies, being completely monotone of order k for all $k \geq m$. We say a function is completely monotone *if it is completely monotone of order $m = 0$.*

This property is easy to verify and can be used to deduce positive definiteness by applying a remarkable property of completely monotone functions, which was first introduced by Bernstein in [Wid46].

Theorem 1.10 (Bernstein-Widder)**.** *The function g is completely monotone on $\mathbb{R}_{>0}$ if and only if it has a representation*

$$g(t) = \int_0^\infty e^{-t\alpha}\, d\mu(\alpha), \quad t > 0, \tag{1.10}$$

as a Laplace transform of a non-decreasing bounded Borel measure μ, that is $d\mu$ non-negative.

Schoenberg showed in [Sch38] the connection between the positive definiteness of the interpolation matrix and the concatenation of the function with the square root being completely monotone.

Theorem 1.11 (Schoenberg)**.** *Let $g(t) \neq const.$ be continuous and completely monotone on $(0, \infty)$; furthermore, let $\Xi \subset \mathbb{R}^d$ be a finite set of distinct points. Then $A_\Xi = \{\phi(\|\xi - \zeta\|)\}_{\xi,\zeta\in\Xi}$, with $\phi(r) = g(r^2)$ is strictly positive definite and nonsingular in any dimension.*

For functions having a first derivative which is completely monotone, Micchelli showed the following extensions (Theorem 2.3 and 2.1, [Mic86]).

Theorem 1.12 (Micchelli 1)**.** *Assume that $g \in C([0, \infty))$, satisfying $g' \neq const$, and g' is completely monotone on $(0, \infty)$. Let also g satisfy $g(0) \geq 0$. Then, for $\phi(r) = g(r^2)$, A_Ξ is non singular for any set of distinct points, $\Xi \subset \mathbb{R}^d$.*

Basis functions derived from this theorem are sometimes referred to as conditionally strictly negative definite functions and for such functions interpolation is possible without a polynomial part added, even though they are not positive definite. The probably best known basis function of this class is the multiquadric. Micchelli also showed that for higher order derivatives the following is true.

Theorem 1.13 (Micchelli 2)**.** *If g is completely monotone of order m and if $g^{(m)}(t) \neq$ const., then $\Phi = \phi(\| \cdot \|) = g(\| \cdot \|^2)$ is strictly conditionally positive definite of order m on $\mathbb{R}^d$ for any $d \in \mathbb{N}$.*

Micchelli's theorem states a sufficient condition for positive definiteness. It took till 1993 until Guo, Hu and Sun proved, that the condition of Micchelli is also necessary (see [GHS93] Theorem 2.1).

Theorem 1.14. *Let $g : \mathbb{R}_{\geq 0} \to \mathbb{R}$ be a continuous function on $[0, \infty)$ and $\Phi(x) = g(\| x \|^2),\ \forall x \in \mathbb{R}^d$, then the following statements are equivalent:*

1. *Φ is conditionally strictly positive definite of order m on $\mathbb{R}^d$ for all $d \in \mathbb{N}$.*

2. *$(-1)^m g^{(m)}$ is completely monotone on $(0, \infty)$.*

With these results, we can show the solvability of the interpolation problem for some of the aforementioned radial basis functions.

Example 1.15.

- *Setting $g(t) = e^{-\alpha t}$, and $t = r^2$, we have the Gaussian radial basis function,*

$$\phi(r) = e^{-\alpha r^2}, \quad \alpha > 0,$$

with

$$g^{(\ell)}(t) = (-1)^\ell \alpha^\ell e^{-\alpha t}, \quad \forall \ell \in \mathbb{N}.$$

Therefore, g is completely monotone for $\alpha > 0$ and $t \in (0, \infty)$. Hence the Gaussian is strictly positive definite.

- *The thin-plate spline,*

$$\phi(r) = r^2 \log(r),$$

is conditionally strictly positive definite of order $m = 2$, because with $g(t) = \frac{1}{2} t \log(t)$ it follows that

$$g''(t) = \frac{1}{2} t^{-1}, \quad t > 0.$$

The given properties are only applicable if the basis function is (conditionally) strictly positive definite for arbitrary dimensions. The Schoenberg and Bernstein theorems only use the underlying function ϕ or g respectively and are dimension independent. Even though functions that are positive definite in arbitrary dimensions are extremely convenient to use, we miss some important classes of radial basis functions, when restricting our research to those. An example of such functions are all functions with zeros. The mentioned criteria by Schoenberg cannot be used to show the solvability properties for radial basis functions ϕ with $\phi(x_0) = 0$, for a specific $x_0 \in \mathbb{R}_{\geq 0}$, because these functions according to Theorem 1.10 satisfy

$$\phi(x_0) = \int_0^\infty e^{-x_0^2 t^2} \, d\mu(t) \neq 0.$$

This includes locally supported radial basis functions like Wendland and Buhmann functions (for example, [Buh03]), as well as oscillatory radial basis functions as described in [FLW06].

To also be able to show the positive definiteness of such functions, and for extensive further use in this thesis, we introduce the concepts of multivariate and generalised Fourier transforms.

Definition 1.16. *Let $f : \mathbb{R}^d \to \mathbb{R}$ be an absolute integrable function, thus $f \in L^1(\mathbb{R}^d)$, then the* Fourier transform *of the function f is given by:*

$$\hat{f}(\xi) = \frac{1}{\sqrt{2\pi}^d} \int_{\mathbb{R}^d} e^{-i\xi^T x} f(x) \, dx, \quad \xi \in \mathbb{R}^d. \tag{1.11}$$

Since we study radial functions for the majority of this thesis, we note here that for radially symmetric functions the inverse-Fourier transform,

$$\check{f}(x) = \frac{1}{\sqrt{2\pi}^d} \int_{\mathbb{R}^d} e^{i\xi^T x} f(x) \, dx, \quad \xi \in \mathbb{R}^d, \tag{1.12}$$

and the Fourier transform are one and the same, so that if $\hat{f} \in L^1(\mathbb{R}^d)$, the Fourier transform is self-invers. Also the Fourier transform of a radially symmetric functions has a special form, which is described in various papers and books, for example [Fas07].

Theorem 1.17. *Given $\Phi \in L^1(\mathbb{R}^d) \cap C(\mathbb{R}^d)$ and $\Phi(x) = \phi(\|x\|)$, $\phi : \mathbb{R} \to \mathbb{R}$. The*

Fourier transform $\hat{\Phi}$ is a radial symmetric function

$$\hat{\Phi}(\xi) = \|\xi\|^{-\frac{d-2}{2}} \int_0^\infty \phi(t) t^{\frac{d}{2}} J_{\frac{d-2}{2}}(\|\xi\| t)\, dt, \tag{1.13}$$

where J_τ denotes the Bessel function of the first kind, given by

$$J_\tau(z) = \sum_{m=0}^{\infty} \frac{(-1)^m (z/2)^{2m+\tau}}{m!\Gamma(m+\tau+1)}. \tag{1.14}$$

We note here that a radial function $\Phi : \mathbb{R}^d \to \mathbb{R}$, $\Phi(x) = \phi(\|x\|)$, satisfies $\Phi \in L^1(\mathbb{R}^d)$ if and only if $t^{d-1}\phi(t) \in L^1(\mathbb{R}_{\geq 0})$.

Theorem 1.18 (Bochner's theorem)**.** *If the Fourier transform of a continuous bounded function $F : \mathbb{R}^d \to \mathbb{R}$, $F \in L^1(\mathbb{R}^d)$, is positive, then the symmetric matrix with entries $F(\xi - \zeta)$, $\xi, \zeta \in \Xi$, is positive definite for all finite sets of distinct points $\Xi \subset \mathbb{R}^d$. For every such function there is a representation of the form*

$$F(x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{ix^T\omega}\, d\mu(\omega), \tag{1.15}$$

where μ is a finite, non-decreasing, Borel measure.

This theorem gives a characterisation of positive definite functions for a fixed dimension d. To characterise also the conditionally positive functions on a given dimension d we will need to extend the concept of the Fourier transform, which we defined for functions in $L^1(\mathbb{R}^d)$, to a more general class of functions. First we will therefore define the concept of the generalised Fourier transform.

Definition 1.19 (Schwartz space)**.** *A function satisfies $\tau \in S(\mathbb{R}^d)$ if and only if $\tau \in C^\infty(\mathbb{R}^d)$ and for all $k \in \mathbb{Z}^d_{\geq 0}$ and for all $\alpha \in \mathbb{Z}^d_{\geq 0}$ the condition:*

$$\left| x^k \frac{\partial^\alpha}{\partial x^\alpha} \tau(x) \right| < C_{\alpha,k}, \quad x \in \mathbb{R}^d,$$

holds. For $m \in \mathbb{N}$ we denote the set of functions $\gamma \in S(\mathbb{R}^d)$ satisfying

$$|\gamma(\omega)| = \mathcal{O}(\|\omega\|^m), \quad \textit{for } \|\omega\| \to 0,$$

by $S_m(\mathbb{R}^d)$.

Definition 1.20. *For a continuous function $\Phi : \mathbb{R}^d \to \mathbb{R}$ which satisfies $|\Phi(x)| = \mathcal{O}(\|x\|^k)$ for $\|x\| \to \infty$ and some $k \in \mathbb{N}$, the generalised Fourier transform $\hat{\Phi} : \mathbb{R}^d \setminus \{0\} \to \mathbb{R}$ is the function satisfying*

$$\int_{\mathbb{R}^d} \Phi(x)\hat{\tau}(x)\,dx = \int_{\mathbb{R}^d} \hat{\Phi}(x)\tau(x)\,dx, \quad \forall \tau \in S_{2m}(\mathbb{R}^d).$$

The smallest such m is called the order of $\hat{\Phi}$. We call $\hat{\Phi}$ a Fourier transform of order m.

The conditionally strictly positive definite functions of order m on $\mathbb{R}^d$ can now be characterised, we take this description from [Wen05].

Theorem 1.21. *Suppose a continuous function $\Phi : \mathbb{R}^d \to \mathbb{R}$ which for some $k \in \mathbb{N}$ satisfies $|\Phi(x)| = \mathcal{O}(\|x\|^k)$ for $\|x\| \to \infty$, has a generalised Fourier transform $\hat{\Phi}$ of order m which is continuous on $\mathbb{R}^d \setminus \{0\}$. Then Φ is conditionally strictly positive definite of order m on $\mathbb{R}^d$ if and only if $\hat{\Phi}$ is non-negative and not identically zero.*

We restrict ourself to introducing only the techniques and definitions necessary to prove the results in the next chapters. For further theoretical results on radial basis function interpolation and quasi-interpolation we refer to the book by Buhmann [Buh03]. For an introduction to the implementation of the radial basis function methods we recommend the book of Fasshauer [Fas07].

1.4 Multiply monotone functions and radial basis functions with compact support

At the end of this chapter we introduce the concept of multiply monotone functions. This concept also allows to give sufficient conditions for the positive definiteness of functions in d-dimensional spaces. Like the two theorems of Micchelli and Guo et al. (quoted as Theorem 1.12 and Theorem 1.14) show the connection between completely monotonicity and positive definiteness of functions, the latter even showing the necessity of the completely monotonicity of $\phi(\sqrt{\cdot})$ for any function that is positive definite on all $\mathbb{R}^d$. We will connect multiply monotonicity and positive definiteness in d dimensions. The proof of such a connection is possible using Bochner's theorem (quoted as Theorem 1.18).

We mention here that the case of conditionally strictly positive definiteness can be ruled out, when investigating functions of compact support. This is because, when applying Bochner's theorem to a function with compact support, its Fourier transform will always be defined and finite in zero.

Multiply monotone functions were first described in the context of radial basis functions by Micchelli and Buhmann in [BM91].

Definition 1.22. *A function f defined on an interval I of reals, also including the full set $I = \mathbb{R}_{\geq 0}$, $f \in C^{\mu-2}(\mathbb{R}_{>0})$, is called μ-times monotone (or multiply monotone) on I if and only if*

$$(-1)^j f^{(j)}(t) \geq 0, \quad \forall\, t \in I,$$

and $(-1)^j f^{(j)}$ is non-increasing and convex for $j = 0, 1, \ldots, \mu - 2$. Here, $\mu > 1$ is an integer. For $\mu = 1$, we require $f \in C(I)$ to be non-negative and non-increasing; then it is called (once) monotone.

In [Wil56] Williamson showed the existence of a representation analogue to the Bernstein-Widder representation for completely monotone functions.

Theorem 1.23. *Every function which is multiply monotone on $\mathbb{R}_{>0}$ has a representation of the form*

$$f(\tau) = \int_0^\infty (1 - \tau\beta)_+^{\lambda-1}\, d\gamma(\beta), \quad \tau > 0, \tag{1.16}$$

where γ is a non-decreasing Borel measure and bounded from below.

To show the connection of positive definiteness and multiple monotonicity, we cite this result from [Fas07] (Theorem 5.5).

Theorem 1.24. *A function $\phi \in C([0,\infty))$ which is n-times monotone on $(0,\infty)$ and is not a polynomial, is strictly positive definite on $\mathbb{R}^d$ for all dimensions d with $n \geq \lfloor d/2 \rfloor + 2$ and $\phi(\|\cdot\|) \in L^1(\mathbb{R}^d)$.*

Multiply monotone functions thereby allow the construction of compactly supported basis functions.

Example 1.25. *The most general multiply monotone function is*

$$\phi(t) = (1-t)_+^k, \quad t \in \mathbb{R}_{\geq 0},$$

it is $k+1$ times monotone on $\mathbb{R}_{\geq 0}$ and therefore positive definite as long as $k-1 \geq \lfloor d/2 \rfloor$. For example $\phi(t) = (1-t)_+^3$ is positive definite on $\mathbb{R}^5$.

The property of multiply monotonicity is not necessary, for example Wendland showed in [Wen96] how to construct compactly supported basis functions, which are usually not multiply monotone. We describe his technique in Appendix A and show that the basis functions constructed are usually derived from multiply monotone functions.

We also already at this point define a concept, that will be of importance mostly in the Chapter 4 of this thesis for the use in spherical interpolation. It is absolute monotonicity.

Definition 1.26. *A function f is called* absolutely monotone *on an interval I of reals if $f \in C^\infty(I)$ and*

$$f^{(n)}(t) \geq 0, \quad \text{for all } n \in \mathbb{N}_0, \quad t \in I.$$

A function f is said to be μ-times absolutely monotone *on I, $\mu \in \mathbb{N}_2$ an integer, if $f \in C^{\mu-2}(I)$ and*

$$f^{(n)}(t) \geq 0, \quad \text{for all } n \leq \mu - 2, \quad t \in I,$$

and $f^{(n)}$ is increasing and convex on I for all such n.

Chapter 2

Generalisations and new results on multiply monotone functions

Completely monotone functions have been studied extensively in the last two decades because they are of use in various fields of mathematical application, there have been new concepts like logarithmically monotonicity introduced and many interesting properties proven. As some examples we refer to the papers [GQ10] and [KM18]. We also saw that in the beginning of the studies about completely monotone functions many authors pointed out the applicability to multiply monotone functions, recent publications often only take into account completely monotone functions. We will therefore transfer the new results on completely monotone and logarithmically monotone functions to multiply monotone functions and generalise the ideas where possible. Many of the results can easily be generalised to the bigger class of multiply monotone functions but one has to dedicate special attention to the orders of monotonicity. We also approach the topic more with a goal of enabling the construction of new multiply monotone functions and testing known functions than describing the relations between the function classes. An approach given in the paper of van Haeringen [vH96].

Also different authors use slightly different definitions of multiply monotonicity, like in [LN83], [vH96] and [Qi05], where the functions are called N-alternating (or n-times monotone) and only have to satisfy

$$(-1)^j g^{(j)} \geq 0, \quad j \leq N+1 \text{ (or } n),$$

resulting in a slightly smaller class of functions (or the multiply monotonicity is restricted to a certain interval). This is the case for the important functions

$$(1-t)_+^{\lambda-1},$$

which according to our definition are λ-times monotone on $[0,\infty)$, but for the other definitions are only $(\lambda-1)$-times monotone because $f^{(\lambda-2)}$ is not continuously differentiable. For the construction of radial basis functions the intervals need to be either $I=\mathbb{R}_{\geq 0}$ or $I=\mathbb{R}_{>0}$ but for the sake of generality and because the intervals $I=[-1,1]$ and $I=[0,\pi]$ will be of importance for spherical basis functions, we will state the results for general intervals where possible.

Many of the first known results on multiply monotone functions were given in the article [Wil56] – who used the same definition as we do, while restricting his definitions and theorems to the case $I=\mathbb{R}_{>0}$. We start this section by stating some of the basic properties he found for general intervals.

Theorem 2.1. *If f is ν-times monotone and g is μ-times monotone on I and $a\in\mathbb{R}_{\geq 0}$, then it is true that*

1. *(af) is ν-times monotone,*
2. *the sum $f+g$ is at least $\min\{\mu,\nu\}$-times monotone,*
3. *the product $f\cdot g$ is at least $\min\{\mu,\nu\}$-times monotone.*

Proof. 1. & 2. follow direct from the definition and 3. follows using the Leibniz rule:

$$(fg)^{(n)}(x)=\sum_{k=0}^{n}\binom{n}{k}f^{(n-k)}(x)g^{(k)}(x).$$

We deduce that

$$(-1)^n(fg)^{(n)}(x)=\sum_{k=0}^{n}\binom{n}{k}(-1)^{n-k}f^{(n-k)}(x)(-1)^k g^{(k)}(x)\geq 0$$

for $n\leq\min\{\mu,\nu\}-2$.

For $n=\min\{\mu,\nu\}-2$ we see that $(-1)^{\min\{\mu,\nu\}-2}(fg)^{\min\{\mu,\nu\}-2}$ is non-increasing because every term of the Leibniz sum is a product of two positive and non-increasing functions and it is convex as a product of two positive, non-increasing and convex functions. $\square$

Williamson also gave another simple characterisation for the class of multiply monotone functions on $\mathbb{R}_{>0}$, which we cite without proof.

Theorem 2.2. *The function $f(t)$ defined for $t > 0$ is μ-times monotone on $\mathbb{R}_{>0}$, $\mu \geq 2$, if and only if*

1. $(-1)^{\mu-2} f^{(\mu-2)}$ *is non-negative, non-increasing and convex on $\mathbb{R}_{>0}$, and*
2. $\lim_{t\to\infty} f(t)$ *exists and is non-negative.*

The following theorem was originally proven in [LN83] for completely monotone functions mentioning the possible generalisation to other monotonicities and also given in [vH96] and in [LMS70] for the more restricted definitions – so we are going to give a proof for the broader class of functions.

Theorem 2.3. *Let a function $g \in C^{\nu-1}(I)$ whose derivative g' is $(\nu-1)$-times monotone on I be given, and another one f which is ν-times monotone on $g(I)$ for $\nu \in \mathbb{N}$, $\nu \geq 2$. Then the composite function $f \circ g$ is ν-times monotone on I.*

Proof. We establish this theorem by induction:
For $\nu = 2$ we know that $f(g(x)) \geq 0$ on $g(I)$, and

$$(-1) f(g(x))' = -g'(x) \cdot f'(g(x)). \tag{2.1}$$

In particular, we have that $g'(x) \geq 0$ is non-increasing and convex, $-f'(g(x)) \geq 0$ is non-increasing (because $g(x)$ is increasing) and convex, so this is also true for the product.

We show that the theorem is true for $\nu + 1$ if it is for ν in order to complete the induction. To this end, we let the function f be $(\nu + 1)$-times monotone and g' be ν-times monotone. Then $f(g(x))$ is non-negative because the function $f(x)$ is non-negative. The derivative of this with an extra minus sign, as in eq. (2.1), is a product of a function g' which is ν-times monotone and $-f'(g(x))$. The last is a composition of the function g and the function $-f'$ which is ν-times monotone, it is therefore ν-times monotone by induction hypothesis. The product in eq. (2.1) is thereby ν-times monotone employing part 3 of the pen-ultimate theorem. □

One special case of the above theorem is given for $I = \mathbb{R}_{\geq 0} = g(I)$ where g' is to be $(\nu - 1)$-times monotone on $\mathbb{R}_{\geq 0}$ and $g(x) \geq 0$ for all $x \in \mathbb{R}_{\geq 0}$. One important example of such a function for arbitrary $\nu \geq 2$ is $g(x) = \sqrt{c^2 + x}$ with $c > 0$.

For completely monotone functions there is the relatively recent terminology of calling a function $g \in C(\mathbb{R}_{\geq 0})$ with $-g'$ completely monotone an almost completely monotone function [Guo16]. We introduce this concept for multiple monotonicity as follows.

Definition 2.4. *A function f is called* almost μ-times monotone *on an interval I if $(-f')$ is $(\mu-1)$-times monotone on I.*

From the last theorem we can deduce many interesting properties which we will later-on connect to the concept of logarithmically monotonicity, to be defined below.

Lemma 2.5. *For this lemma all monotonicity properties are to be on the interval $I = \mathbb{R}_{>0}$.*

1. *If g' is $(\nu-1)$-times monotone, then $(1-g)_+^\alpha$ is ν-times monotone for all $\alpha \geq \nu-1$.*

2. *If the function g is almost ν-times monotone (this is true in particular if g is a ν-times monotone function), then $(g)_+^\alpha$ is ν-times monotone for $\alpha \geq \nu - 1$.*

3. *If the k-th root $\sqrt[k]{g}$ is real valued on $(0,\infty)$ for any non-negative $k \geq \mu$ and μ-times monotone, then g is at least μ-times monotone.*

Proof. We establish these three claims as follows:

1. The first claim follows directly from Theorem 2.3.

2. If $-g'$ is $(\nu-1)$-times monotone, then $h(x) = 1 - g(x)$ satisfies that h' is $(\nu-1)$-times monotone. We furthermore know that the function $(1-\cdot)_+^\alpha$ is $\lfloor\alpha\rfloor + 1$-times monotone. The statement therefore follows from $(g)_+^\alpha = (1-h(x))_+^\alpha$ and from Theorem 2.3.

3. This assertion follows immediately from the previous assertion and from Theorem 2.3.

□

The properties established in this theorem enhance and generalise the results described in [LN83], [vH96], [Guo16] and [GQ10].

It is also easy to establish the possibility of combinations of completely monotone functions and multiply monotone functions. Since every completely monotone function is multiply monotone (μ-times) for arbitrary μ, the above established theorems are also admissible if one function is completely monotone preserving the μ-fold monotonicity of the multiply monotone function.

In the following examples we also use so-called exponential splines, i.e., piecewise exponential functions in place of piecewise polynomials as in ordinary splines (see, e.g., [Ron92]).

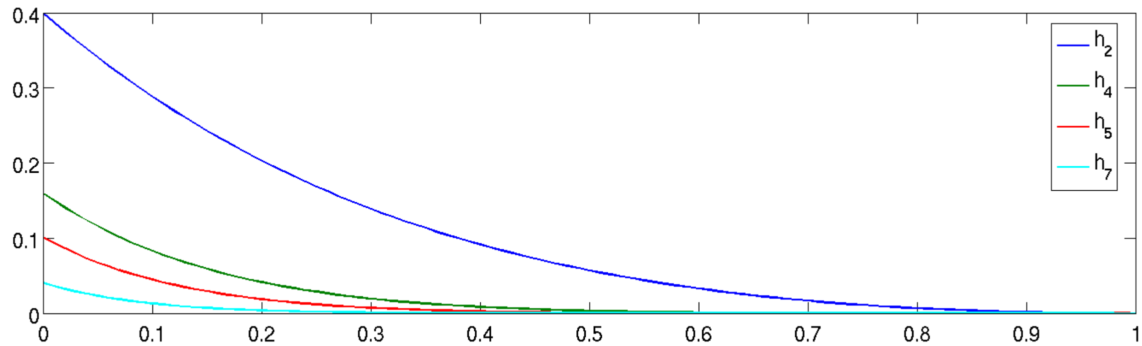

Figure 2.1: The piecewise exponential function of Example 2.6 for $\alpha = 2, 4, 5, 7$.

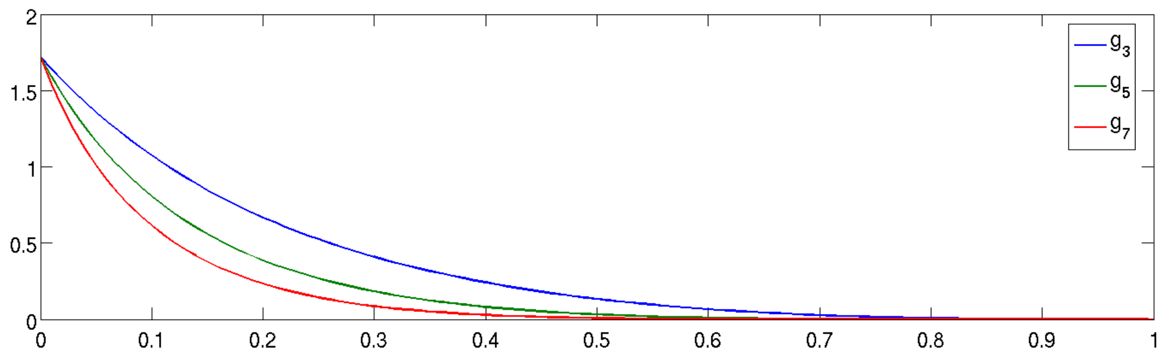

Figure 2.2: The piecewise exponential function of Example 2.7 $g_\alpha = e^{(1-x)_+^\alpha} - 1$ for $\alpha = 3, 5, 7$.

Example 2.6. *The function $h_\alpha(x) = (e^{-x} - e^{-1})_+^\alpha$ is a compactly supported piecewise exponential spline (see Figure 2.1) that is $(\lceil\alpha\rceil + 1)$-times monotone on $\mathbb{R}_{\geq 0}$. For $\alpha = 2$, it is given by*

$$h_2(x) = \begin{cases} e^{-2x} - 2e^{-x-1} + e^{-2}, & x \in [0,1], \\ 0, & x \notin [0,1]. \end{cases}$$

Example 2.7. *The expression $e^{(1-x)_+^\alpha}$, x real, is $(\lceil\alpha\rceil + 1)$-times monotone on $\mathbb{R}_{\geq 0}$, because e^{-x} is completely monotone on $\mathbb{R}$, and because the function $-(1-x)_+^\alpha$ has a derivative which is $\lceil\alpha\rceil$-times multiply monotone. The function itself is not, by the way, of compact support, but this can be easily achieved by subtracting 1 from it. For plots of the resulting functions for several α see Figure 2.2.*

The combination of multiply monotone functions and exponentials is the inspiration for a new concept. We now introduce the notion of the so-called logarithmically monotone functions and define the class of multiply logarithmically monotone functions, a concept also used in [GQ10] – however in the context of completely monotone functions.

Definition 2.8. *Extending all of the aforementioned monotonicity properties, we define the terminology that a positive function $f \in C(I)$ is* logarithmically completely/ ν-times monotone *as follows: The function $f \in C(I)$ is* logarithmically ν-times monotone *(where we take $\nu \in \mathbb{N}$, $\nu \geq 2$) if and only if the non-negative expression*

$$(-1)^{\ell}\Big(\log(f)\Big)^{(\ell)}(x) \geq 0, \qquad \forall\, x \in I, \tag{2.2}$$

is non-increasing and convex for $\ell = 1, 2, \ldots, \nu-2$. Further, the function is logarithmically 2-times (twice) monotone *if* $\log(f)$ *is non-increasing and convex. Finally, we call $f \in C(I)$* logarithmically completely monotone *if our displayed condition holds for all $\ell \in \mathbb{N} \setminus \{0\}$.*

We can next give a description of logarithmically multiply monotone functions that also holds for logarithmically completely monotone functions and which was also given in [vH96] for $I = \mathbb{R}_{>0}$.

Theorem 2.9. *A function $f : \mathbb{R} \to \mathbb{R}$ is logarithmically μ-times monotone on I if and only if it is positive and f^{α} is μ-times monotone on I for every positive α.*

Proof. We consider the different possible choices of μ separately as shown in the subsequent list.

1. We start with $\underline{\mu = 2}$. In that instance, because f is logarithmically twice monotone, it is straightforward that the asserted equivalence between $f(x)$ being positive for all $x \in I$ and the existence of $\log(f)$ for all $x \in I$ holds. Moreover, it is also equivalent that $\log f$ is non-increasing and that f^{α} is non-increasing for all $\alpha > 0$.

   Furthermore, it is true that the convexity of $\log f$ and the convexity f^{α} for all positive powers α are equivalent, this follows from the Hurwitz representation

   $$\log(f(x)) = \lim_{n\to\infty} n \left(\sqrt[n]{f(x)} - 1 \right).$$

2. We consider next all the other cases $\underline{\mu > 2}$. Those remaining cases are treated as follows:

   ⇒ Let f be logarithmically μ-times monotone on $\mathbb{R}_{\geq 0}$, i.e. $g = \log(f)$ is almost μ-times monotone. Then it follows that f^{α} is μ-times monotone, due to the identity $f^{\alpha} = \exp(\alpha g)$ and by Theorem 2.3.

$\Leftarrow$ We use the identity

$$-(\log f)' = -\lim_{\alpha \to 0} f^{\alpha-1} f' = -\lim_{\alpha \downarrow 0} \frac{1}{\alpha} (f^{\alpha})',$$

and we use also that the power f^{α} is μ-times monotone too. This therefore holds for the limit as well.

The theorem is proved. $\square$

Theorem 2.10. *It is a consequence of the above theorem that the logarithmically monotonicities are stronger than first defined monotonicity concepts. In other words, every logarithmically completely/ multiply monotone function is also completely/ multiply monotone. The converse is not true.*

Proof. The first statement follows immediately from our work. We give the counterexample for the last statement

$$f(x) = (1-x)_{+}^{\beta},$$

with a power $\beta \geq 3$. The logarithm of this functions is not defined for $x \geq 1$ and therefore it is not logarithmically monotone of any order. $\square$

The following interesting theorem was given for absolute monotone functions in the fundamental paper by Widder [Wid46] for the interval $I = \mathbb{R}_{>0}$ and general $g(I)$.

Theorem 2.11. *If the function f is μ-times absolute monotone on $g(I)$ and $-g'$ is $(\nu-1)$-times monotone on I, then the composition $f(g(x))$, $x \in \mathbb{R}$, is at least* $\min\{\mu, \nu\}$*-times monotone on $g(I)$.*

Proof. The proof follows using the argument that, for every function f that is absolute monotone on $g(I)$, the function $f(-\cdot)$ is multiply monotone on $-g(I)$. Now, replacing g by $-g$ yields the statement by employing Theorem 2.3. $\square$

Lemma 2.12. *If, in the above theorem, g is multiply monotone of order ν, then it is sufficient that f is absolute monotone of order μ on $[0, \infty)$, so that $f(g)$ is* $\min\{\mu, \nu\}$*-times monotone.*

From the last theorems, we can easily deduce these special cases.

Lemma 2.13.

1. *If a function g is ν-times monotone, then the power $(g)^{\alpha}$ for positive α is* $\min\{\lfloor \alpha \rfloor, \mu\}$*-times monotone, whereas for the truncated power $(g)_{+}^{\alpha}$ with positive α to be multiply monotone it is sufficient that the derivative $-g'$ is $(\mu-1)$-times monotone.*

2. *If $-g'$ is $(\nu-1)$-times monotone on I, then the function $e^{g(\cdot)}$ is multiply monotone of order ν on I.*

3. *If $\log(g(\cdot))$ exists and is ν-times monotone on I, then so is g.*

Example 2.14. *We show that the function*

$$f_{\alpha,\beta}(x) = (1+\alpha x)_+^{\beta}, \quad x \geq 0, \tag{2.3}$$

gives, for different values of α and β, examples for most of the described monotonicities; they are taken all along the half-line $\mathbb{R}_{\geq 0}$.

- *For positive α and positive β, but $\beta \notin \mathbb{N}$, the function is $(\lfloor\beta\rfloor+1)$-times absolute monotone.*

- *For positive α and $\beta \in \mathbb{N}$, the function is absolutely monotone.*

- *For $\alpha = \frac{1}{n}$ and $\beta = n$, the limit*

$$\lim_{n\to\infty} f_{\alpha,\beta}(x) = \lim_{n\to\infty} f_{1/n,n}(x) = \exp(x)$$

  is absolutely monotone.

- *For negative α and positive β, the function we generate is $(\lfloor\beta\rfloor+1)$-times monotone.*

- *For $\alpha = -\frac{1}{n}$ and $\beta = n$,*

$$\lim_{n\to\infty} f_{\alpha,\beta}(x) = \lim_{n\to\infty} f_{-1/n,n}(x) = \exp(-x)$$

  is logarithmically completely monotone.

- *For positive α and negative β, the function f is logarithmically completely monotone.*

Some new results were published in Feng Qi [Qi05] who also used the more specific definition of monotone functions; we give an alternative proof. The results are:

Theorem 2.15. 1. *For a differentiable function h, whose first derivative h' is $(\mu-1)$-times monotone on I, and for which f is logarithmically ν-times monotone on $h(I)$, it follows that $f(h(x))$ is logarithmically $\min\{\mu,\nu\}$-times monotone on I.*

2. *For a function $f : \mathbb{R} \to \mathbb{R}$ that is logarithmically μ-times monotone on $\mathbb{R}_{>0}$, the function*
$$g(x) = \frac{f(x)}{f(x+\alpha)}, \tag{2.4}$$
with positive α, is logarithmically $(\mu - 1)$-times monotone on $\mathbb{R}_{>0}$.

Proof. We establish our claims item by item:

1. We know that $g = \log(f)$ is almost ν-times monotone and that $-g'$ is $(\nu - 1)$-times monotone.

   Now $-(\log(f(h)))' = -(g(h))' = -g'(h) \cdot h'$ using Theorem 2.3, and furthermore using that the product of two $(\mu - 1)$-times and $(\nu - 1)$-times monotone functions, respectively, is $(\min\{\mu, \nu\} - 1)$-times monotone, we conclude that the composition $f(h)$ is logarithmically $\min\{\mu, \nu\}$-times monotone.

2. Since f is logarithmically μ-times monotone, we have that
$$-(\log(f))'$$
   is $(\mu - 1)$-times monotone. Therefore, it is enough to show that
$$-\log\left(\frac{f(x)}{f(x+\alpha)}\right)'$$
   is $(\mu-2)$-times monotone for a non-negative α. We do this by applying Theorem 2.2.

   We know that, $\mu \geq 3$,
$$G(x) = (-1)^{\mu-3}\Big(\log(f(x)\Big)^{(\mu-3)}$$
   is non-negative and non-increasing. Therefore we get the inequality
$$0 \leq (-1)^{\mu-3}(\log(f(x+\alpha))^{(\mu-3)} \leq (-1)^{\mu-3}(\log(f(x))^{(\mu-3)}.$$
   We conclude that
$$\begin{aligned}(-1)^{\mu-3}&\left(\log\left(\frac{f(x)}{f(x+\alpha)}\right)\right)^{(\mu-3)} \\ &= (-1)^{\mu-3}\left(\log(f(x))^{(\mu-3)} - (\log(f(x+\alpha))^{(\mu-3)}\right)\end{aligned}$$

is non-negative. To further prove that $G(x)$ is non increasing and convex by using the $(\mu-2)$-nd derivative of $\log(f)$. We know that

$$h(x) = (-1)^{\mu-2}\Big(\log(f(x)\Big)^{(\mu-2)}$$

is positive, non-increasing and convex because f is μ-time logarithmically monotone. For the $(\mu-2)$-nd derivative of the function of interest we get

$$(-1)^{\mu-2}\left(\log\left(\frac{f(x)}{f(x+\alpha)}\right)\right)^{(\mu-2)} = (-1)^{\mu-2}\left(h(x) - h(x+\alpha)\right)$$

and from h being non increasing it follows that the above is non negative and from h being convex it follows that the above is non-increasing. To proceed and apply Theorem 2.2 we need to show the existence of the limit, we know that $\lim\limits_{x\to\infty} -\Big(\log(f(x))\Big)'$ exists and is non-negative. We can therefore finally remark that

$$\lim_{x\to\infty} -\left(\log\left(\frac{f(x)}{f(x+\alpha)}\right)\right)'$$

exists and is zero for all α.

□

Finally we generalise the result recently described in [Guo16] and [KM18], which was, however, not stated there for multiply monotone functions and general intervals.

Theorem 2.16. *If $f \in C(I)$ and if it is positive on I, and if f' is $(\mu-1)$-times monotone on I, then $\frac{1}{f}$ is μ-times logarithmically multiply monotone on the interval I.*

Proof. We know that $(\cdot)^{-1}$ is completely monotone on the strictly positive half-axis, and therefore we can conclude, using Theorem 2.3, that $\frac{1}{f}$ is multiply monotone of order μ. For the logarithm we know that $\log(f^{-1}) = -\log(f)$ and that therefore $-\left((\log(f^{-1}))\right)' = \frac{1}{f}\cdot f'$. We can deduce that the latter is $(\mu-1)$-times monotone as a product of functions which are at least $(\mu-1)$-times monotone. □

We see in the last two theorems, that the concept of logarithmically monotonicity is extremely helpful in determining the monotonicity properties of rational functions. It is in those cases easier to prove than complete monotonicity. To show this we give three examples, the first one was first described by Mehrez in [Meh15], Theorem 1.

Example 2.17. *Let* $0 < q < 1$ *and* $0 < a < b$. *Then the function* $\frac{\Gamma_q(ax)^\alpha}{\Gamma_q(bx))^\beta}$ *is logarithmically completely monotone on* $(0, \infty)$ *if and only if* $\alpha \geq 0$ *and* $\alpha a = \beta b$. *The q-gamma function is defined by*

$$\Gamma_q(x) = (1-q)^{1-x} \prod_{n=0}^{\infty} \frac{1-q^{n+1}}{1-q^{n+x}}.$$

Example 2.18. *In [KM18] the authors showed that the function*

$$f(t) = \frac{1}{t^{\frac{\alpha+1}{2}} K_\alpha(\sqrt{t})}, \qquad t \in (0, \infty),$$

is logarithmically completely monotone on $(0, \infty)$ *for* $\alpha > 0$.

Example 2.19. *The function*

$$f(x) = \frac{1}{c^2 - (1-ax)_+^{\mu-1}}, \quad c > 1,$$

is μ*-times logarithmically monotone.*

The merit of the above method lies in the transformation of the fraction into a difference by the logarithm. We are therefore also interested studying differences of multiply monotone functions. The following difference operator was suggested by Porcu in the context of smoothing radial basis functions, to be precise for a special case of Buhmann functions [ZP17] but it can also be used to derive new multiply monotone functions.

Theorem 2.20. *Let* f *be a* μ*-times monotone function on* $\mathbb{R}_{\geq 0}$. *Then we have that*

$$g(x) := \beta_2^\varepsilon f\Big(\frac{x}{\beta_2}\Big) - \beta_1^\varepsilon f\Big(\frac{x}{\beta_1}\Big), \qquad \varepsilon > 0, \quad \beta_2 > \beta_1 > 0, \tag{2.5}$$

is $\min\{\mu - 2, \lfloor \varepsilon \rfloor\}$*-times monotone on* $\mathbb{R}_{\geq 0}$.

Proof. Forming the derivative of g we find that

$$(-1)^n g^{(n)}(x) = (-1)^n \left(\beta_2^{\varepsilon - n} f^{(n)} \left(\frac{x}{\beta_2} \right) - \beta_1^{\varepsilon - n} f^{(n)} \left(\frac{x}{\beta_1} \right) \right).$$

Furthermore, for $n \leq \varepsilon$, we know that $\beta_2^{\varepsilon - n} \geq \beta_1^{\varepsilon - n}$ and because $(-1)^n f^{(n)}(x)$ is positive and is non increasing for $n \leq \mu - 2$, we have

$$(-1)^n f^{(n)} \left(\frac{x}{\beta_2} \right) \geq (-1)^n f^{(n)} \left(\frac{x}{\beta_1} \right).$$

This gives therefore $(-1)^n g^{(n)}(x) \geq 0$ for all $n \leq \min\{\mu - 2, \lfloor \varepsilon \rfloor\}$. □

We establish another difference operator which is of special use for functions which are completely monotone of order k.

Theorem 2.21. *Let f be a function which is completely monotone of order k. Then the function*

$$f_{a,b}(x) = f(x+a) - f(x+b), \ \ a > b > 0 \tag{2.6}$$

is completely monotone of order $k-1$.

Proof. The derivatives of $f_{a,b}$ are given as,

$$f_{a,b}^{(\ell)}(x) = f^{(\ell)}(x+a) - f^{(\ell)}(x+b)$$

we now deduce for $\ell \geq k-1$

$$\begin{aligned}
(-1)^\ell f_{a,b}^{(\ell)}(x) &= (-1)^\ell \left(f^{(\ell)}(x+a) - f^{(\ell)}(x+b)\right) \\
&= (-1)^\ell \left(-f^{(\ell)}(x+b) - \int_{x+a}^{x+b} f^{(\ell+1)}(t)dt + f^{(\ell)}(x+b)\right) \\
&= (-1)^{\ell+1} \int_{x+a}^{x+b} f^{(\ell+1)}(t)dt \geq 0.
\end{aligned}$$

The last equation holds because f is completely monotone of order k and therefore

$$(-1)^\ell f^{(\ell)}(x) \geq 0,$$

for all $\ell \geq k$. □

We finally give some other examples of basis functions constructed using the results of this section.

Example 2.22. *1. The function $\phi(x) = e^{-\|x\|^\beta}$, $x \in \mathbb{R}^d$, is positive definite in every dimension d for $0 < \beta \leq 2$, because $f(x) = g(x^2)$ with $g(t) = e^{-t^{\beta/2}}$. We observe that the latter function is indeed completely monotone using Theorem 2.11.*

2. The function

$$\phi(x) = e^{(1-\|x\|)_+^{\lambda-1}} - 1, \qquad x \in \mathbb{R}^d,$$

with the integer $\lambda \in \mathbb{N}$ at least two, is positive definite in every dimension $d \leq 2\lambda - 4$.

3. *The function* $f(t) = 2 - (1-t)_+^{\mu+1}$ *is positive on* $\mathbb{R}^d$ *and the derivative* $f'(t) = (\mu+1)(1-t)_+^{\mu}$ *is* $(\mu+1)$*-times monotone. Therefore, using Theorem 2.16, we get that*
$$\phi(x) = \frac{1}{2-(1-\|x\|)_+^{\mu+1}} - \frac{1}{2},$$
is positive definite on $\mathbb{R}^d$ *for* $d \leq 2\mu - 2$*.*

4. *Even though the truncated power is not logarithmically monotone we can construct logarithmically monotone functions with it. Form the above example and Theorem 2.15 we deduce that*
$$\phi(x) = \frac{c^2-(a-\|x\|)_+^{\mu+1}}{c^2-(1-\|x\|)_+^{\mu+1}} - 1, \quad c > 1, \quad 0 < a < 1,$$
is positive definite on $\mathbb{R}^d$ *for* $d \leq 2\mu - 4$*.*

5. *Using Theorem 2.21 it is easy to establish the positive definiteness of the function*
$$\phi(x) = \log\left(\frac{\|x\|^2+a^2}{\|x\|^2+b^2}\right), \quad a > b.$$

Chapter 3

Construction of radial basis functions

This chapter is divided into three parts. We start by showing how the multiply monotone functions described in the last section can be used to construct radial basis functions which are positive definite but not necessarily multiply monotone.

In the second section we concentrate on shifts of radial basis functions. We where possible prove their positive definiteness, determine an integral representation and compute their Fourier transform. In the last section we will study a class of radial basis functions which are derived as the inverse Fourier transform of a generalisation of the Gaussian basis functions.

3.1 Radial basis functions as Fourier transforms of multiply monotone functions

There are several ways to construct positive definite functions from multiply monotone functions. In addition to the one we will now describe, there are the well-known dimension-walk methods initiated by Wendland, which allow the construction of smooth compactly supported basis functions from multiply monotone functions (for detail see Appendix A). Of course the multiply monotone functions can be directly used as positive definite radial basis functions as a result of the theorem by Micchelli and Buhmann (cited as Theorem 1.24).

We now want to add a way of constructing positive definite radial basis functions which will not be multiply monotone themselves but are Fourier transforms of multiply monotone functions.

Theorem 3.1. *Let g be a k-times monotone function on the non-negative real half-axis and $g(x^2) \in L^1(0,\infty)$. Then the cosine transform, i.e. the Fourier integral along the half-line with only its real, symmetric* cos*-part times two, called $\phi = \hat{f}^c$ of $f(x) := g(x^2)$ is a positive definite kernel on the d-dimensional real space, for all d at most $2k+1$.*

Proof. The symmetry of the cosine transform gives

$$\phi(t) := \hat{f}^c(t) = \sqrt{\frac{2}{\pi}} \int_0^\infty \cos(xt) g(x^2)\, dx, \qquad t \geq 0. \tag{3.1}$$

Because g is k-times multiply monotone, we can represent $f(x) = g(x^2)$ using Theorem 1.23 as

$$f(x) = \int_0^\infty (1 - \beta x^2)_+^{k-1}\, d\mu(\beta), \qquad x \geq 0,$$

the measure having the usual properties. We begin with simplifying the function ϕ, using (12.34.10) from [GR14]:

$$\begin{aligned}
\phi(x) &= \sqrt{\frac{2}{\pi}} \int_0^\infty \cos(xt) \int_0^\infty \left(1 - \beta t^2\right)_+^{k-1} d\mu(\beta)\, dt \\
&= \sqrt{\frac{2}{\pi}} \int_0^\infty \beta^{k-1} \int_0^\infty \cos(xt) \left(\beta^{-1} - t^2\right)_+^{k-1} dt\, d\mu(\beta) \\
&= \sqrt{\frac{2}{\pi}} \int_0^\infty \beta^{k-1} 2^{k-1} \Gamma(k) \beta^{-k/2+1/4} x^{-k+1/2} J_{k-1/2}\Big(\sqrt{\frac{1}{\beta}} x\Big)\, d\mu(\beta).
\end{aligned}$$

We are allowed to exchange the integrals in the above equations because $g(x^2) \geq 0$ and $g(x^2) \in L^1(0,\infty)$.

We now show that the interpolation matrices derived from such radial basis functions are strictly positive definite. This is the case because, for a non-vanishing set of coefficients c_ξ, $\xi \in \Xi \subset \mathbb{R}^{2k+1}$, we have the quadratic form – by the definition of the Bessel functions as

$$\frac{J_{k-\frac{1}{2}}(\|x\|)}{\|x\|^{k-\frac{1}{2}}} = \frac{1}{(2\pi)^{k+\frac{1}{2}}} \int_{\mathbb{S}^{2k}} \exp(i\omega^T x)\, d\omega,$$

where the last integral is the surface integral over the unit sphere in $\mathbb{R}^{2k+1}$ (from [Buh03, p.53]), thus we conclude

$$\sum_{\xi\in\Xi}\sum_{\zeta\in\Xi} c_\xi c_\zeta \phi(\|\xi-\zeta\|) = \sum_{\xi\in\Xi}\sum_{\zeta\in\Xi} c_\xi c_\zeta \sqrt{\frac{2}{\pi}} \int_0^\infty \beta^{k/2-3/4} 2^{k-1}\Gamma(k)(\|\xi-\zeta\|)^{-k+1/2}$$
$$J_{k-1/2}\Big(\sqrt{\frac{1}{\beta}}\|\xi-\zeta\|\Big)\, d\mu(\beta)$$
$$= \frac{2^{k-1/2}\Gamma(k)}{\sqrt{\pi}} \sum_{\xi\in\Xi}\sum_{\zeta\in\Xi} c_\xi c_\zeta \int_0^\infty \frac{J_{k-1/2}\Big(\sqrt{\frac{1}{\beta}}\|\xi-\zeta\|\Big)}{\beta^{1/2}\left(\sqrt{\frac{1}{\beta}}\|\xi-\zeta\|\right)^{k-1/2}}\, d\mu(\beta)$$
$$= \frac{\Gamma(k)}{2\pi^{k+\frac{1}{2}}} \sum_{\xi\in\Xi}\sum_{\zeta\in\Xi} c_\xi c_\zeta \int_0^\infty \beta^{-1/2}$$
$$\int_{\|\omega\|=1} \exp\left(i\omega^T(\xi-\zeta)/\sqrt{\beta}\right)\, d\omega\, d\mu(\beta)$$
$$= \frac{\Gamma(k)}{2\pi^{k+\frac{1}{2}}} \int_0^\infty \sqrt{\frac{1}{\beta}}$$
$$\int_{\|\omega\|=1} \left|\sum_{\xi\in\Xi} c_\xi \exp\left(i\omega^T\xi/\sqrt{\beta}\right)\right|^2 d\omega\, d\mu(\beta) \geq 0.$$

The above is non-zero by the linear independence of different imaginary powers of the exponential functions – the centres of the interpolation problem always being distinct – thus in fact positive unless all coefficients vanish, the non-negativity having been established before, as required. □

The condition that the function g has to be multiply monotone is in fact weaker than f being multiply monotone because applying Theorem 2.3 multiply monotonicity of f implies multiply monotonicity of $g(\cdot) = f\left(\sqrt{\cdot}\right)$.

In the above theorem we are only able to construct functions which are positive definite up to an odd dimension. If we want to generalise the concept for even dimensions we need to introduce a generalisation of multiple monotonicity which was also defined by Williamson in [Wil56].

Definition 3.2. *The function $f : \mathbb{R}_{>0} \to \mathbb{R}$ is α-times monotone for $\alpha \in \mathbb{R}$, $\alpha \geq 1$ if it can be expressed in the form*

$$f(t) = \int_0^\infty (1-ut)_+^{\alpha-1} d\gamma(u), \quad t > 0, \tag{3.2}$$

where $\gamma(u)$ is non-decreasing and $\gamma(0) = 0$.

This class satisfies monotonicity conditions for the fractional derivative (as introduced by Riemann-Liouville) defined by

$$D^{-\beta+n}f(t) = \frac{\partial^n}{\partial t^n}\frac{1}{\Gamma(\beta)}\int_0^t (t-u)^{\alpha-1}f(u)du, \tag{3.3}$$

where $0 \leq \beta < 1$, $n \in \mathbb{N}$.

To show one of the favourable properties of this definition of the fractional derivative we state the following lemma.

Lemma 3.3. *The presented form of the fractional derivative satisfies*

$$\left(D^{-\beta+n}f\right)^{\wedge}(t) = (+it)^{-\beta+n}\,\widehat{f}(t), \quad n \in \mathbb{Z}_{\geq 0}, \quad 0 \leq \beta < 1.$$

Proof. We know that

$$\left(D^{-\beta+n}f\right)^{\wedge}(s) = \frac{1}{\Gamma(\beta)\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ist}\frac{\partial^n}{\partial t^n}\int_0^t (t-u)^{\beta-1}f(u)du\,dt.$$

Applying integration by parts n-times we get

$$\begin{aligned}
\left(D^{-\beta+n}f\right)^{\wedge}(s) &= \frac{(is)^n}{\Gamma(\beta)\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ist}\left(\int_0^t (t-u)^{\beta-1}f(u)\,du\right)dt \\
&= \frac{(is)^n}{\Gamma(\beta)\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ist}\left(\int_0^1 (1-u)^{\beta-1}t^{\beta}f(tu)\,du\right)\,dt \\
&= \frac{(is)^n}{\Gamma(\beta)\sqrt{2\pi}}\int_0^1 (1-u)^{\beta-1}\left(\int_{-\infty}^{\infty} e^{-ist}t^{\beta}f(tu)\,dt\right)\,du \\
&= \frac{(is)^n}{\Gamma(\beta)\sqrt{2\pi}}\int_0^1 (1-u)^{\beta-1}\frac{1}{u^{\beta+1}}\int_{-\infty}^{\infty} e^{-ist/u}t^{\beta}f(t)\,dt\,du \\
&= \frac{(is)^n}{\Gamma(\beta)\sqrt{2\pi}}\int_{-\infty}^{\infty} t^{\beta}f(t)\left(\int_0^1 (1-u)^{\beta-1}\frac{1}{u^{\beta+1}}e^{-ist/u}\,du\right)\,dt \\
&= \frac{(is)^n}{\Gamma(\beta)\sqrt{2\pi}}\int_{-\infty}^{\infty} t^{\beta}f(t)\int_1^{\infty}\frac{(u-1)^{-\beta+1}}{1}e^{-istu}\,du\,dt.
\end{aligned}$$

Applying [GR14], (3.382.2) to the inner integral of the above equation we can prove:

$$\begin{aligned}\left(D^{-\beta+n}f\right)^{\wedge}(s) &= \frac{(is)^n}{\Gamma(\beta)\sqrt{2\pi}}\int_{-\infty}^{\infty} t^{\beta} f(t)(ist)^{-\beta} e^{-ist}\Gamma(\beta)\,dt \\ &= (+is)^{-\beta+n}\,\widehat{f}(s).\end{aligned}$$

□

The α-times monotone functions can be characterised as functions satisfying the following monotonicity condition (the result is cited from Williamson [Wil56] without proof):

1. $D^{\alpha-2}[t^{\alpha-1}f(\frac{1}{t})]$ is non-negative non decreasing and convex for $t > 0$
2. and $\lim_{t\to\infty} f(t)$ exists and is non-negative.

Remark 3.4. *We note that since Williamson proved that α-times monotonicity implies β-times monotonicity for all $\beta < \alpha$ the derivatives of an α-times monotone function satisfy the know sign changing property of an $\lfloor\alpha\rfloor$-times monotone function.*

We can now derive functions which are positive definite up to an even dimension.

Theorem 3.5. *Let g be a $\left(k+\frac{1}{2}\right)$-times monotone function on the non-negative real half-axis and $g(x^2) \in L^1(0,\infty)$. Then the cosine transform, $\phi = \hat{f}^c$ of $f(x) := g(x^2)$ (as in eq.* (3.1)*) is a positive definite kernel on the d-dimensional real space, for all $d \leq 2k+2$.*

Proof. The proof follows from the proof of Theorem 3.1 by replacing $k \mapsto k + \frac{1}{2}$. □

Example 3.6. *This theorem can be used to derive new radial basis functions, where the simplest example would be the function class*

$$s^{1/2-k} J_{k-1/2}(s)$$

on the non-negative reals. This is the special case of eq. (3.1) *where $\mu(\beta) = (\beta-1)_+^0$ thus $\mu'(\beta) = \delta(\beta-1)$. Here, the spatial dimension could be up to $2k+1$. This function has been considered, albeit with a different derivation, first for interpolation in $\mathbb{R}^d$ by [FLW06], where they also show favourable properties when the basis function is scaled to become increasingly flat. It was also considered for cardinal-interpolation by [Fly06], who showed polynomial reproduction of the cardinal interpolant. Further radial basis functions can be derived using this theorem and are therefore expected to give good numerical results when used for interpolation, cardinal interpolation or quasi-interpolation.*

Example 3.7. *The theorem also allows to identify the positive definiteness of other functions in a simple way. As an example we show the positive definiteness of the Matern kernel, which of course has already been shown in other ways. The Matern kernel is frequently used in statistics and probability theory. The Kernel can be represented as*

$$\phi(x) = x^\tau K_\tau(x) = \frac{2^\tau}{\sqrt{\pi}}\Gamma\Big(\tau + 1/2\Big)\int_0^\infty \cos(xt)(t^2+1)^{-\tau-1/2}\,dt$$

with $R(\tau) \geq \frac{1}{2}$ (see [AS72] 9.6.25). By setting $g(t) = \Gamma(\tau+1/2)2^{\tau-1/2}(t+1)^{-\tau-1/2}$ we can deduce using Theorem 3.1 that ϕ is positive definite on $\mathbb{R}^d$ for any d, because g is completely monotone.

3.2 Shifts of radial basis functions

One of the most commonly used radial basis function is the multiquadric

$$\phi(r) = (r^2 + c^2)^\beta, \qquad \beta \notin \mathbb{Z}_{\geq 0}.$$

The multiquadric can be interpreted as a shift of the linear radial basis function $\phi(r) = r^{2\beta}$, so long as $\beta > 0$. The parameter c is then used as a smoothing parameter. In many applications and tests introducing a smoothing parameter led to better results than the original basis function, as for example described by the author et al. in [JKBS16]. We wanted to investigate whether a generalisation of this concept to a bigger set of radial basis functions is possible and under which conditions the positive definiteness is preserved by the shift. We define the shifts of radial basis functions by the parameter $c \in \mathbb{R}$, via

$$\Phi_c(x) = \phi_c(\|x\|) = \phi(\sqrt{\|x\|^2 + c^2}). \tag{3.4}$$

Those shifts are standard, for multiquadrics $\phi_c(\|x\|) = \sqrt{\|x\|^2 + c^2}$, viewed as a shift of $\phi(\|x\|) = \|x\|$ and they are common for thin-plate splines too.

3.2.1 Shifts of conditionally positive definite functions

For every radial basis function ϕ being representable through $\phi(\|x\|) = g(\|x\|^2)$, as presented in Theorem 1.14, the shifted version can be described by

$$\phi_c(\|x\|) = g(\|x\|^2 + c^2). \tag{3.5}$$

This allows us to easily deduce positive definiteness properties for such functions using the results of Section 1.3. We start with functions which are positive definite in arbitrary dimensions.

Theorem 3.8. *Let ϕ be a strictly positive definite function for all $\mathbb{R}^d$, $d \in \mathbb{N}$, then $\phi_c(\|x\|) = g_c(\|x\|^2)$ is strictly positive definite as well and its Bernstein representation is*

$$g_c(t) = \int_0^\infty e^{-t\alpha}\, d\mu_c(\alpha), \qquad t > 0, \tag{3.6}$$

with $d\mu_c(\alpha) = e^{-c^2\alpha}\, d\mu(\alpha)$. Here μ is the finite Borel measure used in the Bernstein representation of $g(t) = \phi(\sqrt{t})$.

Proof. Since ϕ is positive definite for any dimension d we can apply Theorem 1.14 and

Theorem 1.10 to show that $\phi(\|x\|) = g(\|x\|^2)$, with $g(t) = \int_0^\infty e^{-t\alpha} d\mu(\alpha)$, for $t > 0$. Using the above definition, $g_c(t) = g(t + c^2)$, therefore gives

$$g_c(t) = g(t + c^2) = \int_0^\infty e^{-(t+c^2)\alpha}\, d\mu(\alpha) = \int_0^\infty e^{-t\alpha} \underbrace{e^{-c^2\alpha}\, d\mu(\alpha)}_{=d\mu_c(\alpha)}$$

and from $d\mu$ being a positive non decreasing measure and $e^{-c^2\alpha} > 0$ for all α, it follows that $d\mu_c$ is likewise non decreasing and positive. Therefore g_c is completely monotone implying ϕ_c to be strictly positive definite according to Theorem 1.11. □

There is a representation similar to Bernstein's for conditionally strictly positive definite functions of order 1. It was introduced by Micchelli and is an immediate consequence of (1.10). For this as well, it is possible to show the connection between the shift and the defining measure.

Theorem 3.9. *Given a conditionally strictly positive definite function of order* 1 *and its representation*

$$\phi(r) = \phi(0) - \int_0^\infty \frac{1 - e^{-r^2 t}}{t}\, d\mu(t), \quad r > 0,$$

then $\phi_c(r) = \phi(\sqrt{r^2 + c^2})$ *is conditionally strictly positive definite of order* 1 *with*

$$\phi_c(r) = \phi_c(0) - \int_0^\infty \frac{1 - e^{-r^2 t}}{t}\, d\mu_c(t), \qquad r > 0, \tag{3.7}$$

where $d\mu_c(t) = e^{-c^2 t}\, d\mu(t)$.

Proof. Since we can express ϕ_c using the above representation of ϕ

$$\begin{aligned}
\phi_c(r) &= \phi(\sqrt{r^2 + c^2}) \\
&= \phi(0) - \int_0^\infty \frac{1 - e^{-r^2 t} \cdot e^{-c^2 t}}{t}\, d\mu(t) \\
&= \phi(0) - \int_0^\infty \frac{1 - e^{-c^2 t}}{t}\, d\mu(t) - \int_0^\infty \frac{1 - e^{-r^2 t}}{t} e^{-c^2 t}\, d\mu(t) \\
&= \phi_c(0) - \int_0^\infty \frac{1 - e^{-r^2 t}}{t}\, d\mu_c(t)
\end{aligned}$$

and since $d\mu$ is a positive non decreasing measure, we conclude, using $e^{-c^2\alpha} > 0$ for all α, $d\mu_c \geq 0$ as well as non decreasing. □

Lemma 3.10. *For every function g that is completely monotone of order m the function $g_c(t) = g(t + c^2)$ is completely monotone of order m.*

Proof. For every g the derivatives of g_c are

$$g_c^{(\ell)}(t) = g^{(\ell)}(t + c^2), \text{ for all } \ell \in \mathbb{N}.$$

We conclude if g is completely monotone of a certain order then so is g_c. □

Example 3.11. *1. We can easily deduce from Theorem 1.14 that the linear $\phi(r) = r^{2\beta}$, $\beta > 0,\ \beta \notin \mathbb{N}$ is conditionally strictly positive of order $\lceil \beta \rceil + 1$. Knowing that the generalised multiquadric,*

$$\phi_c(r) = \left(r^2 + c^2\right)^{\beta/2},$$

is the shift of the linear we can deduce that the multiquadric is conditionally strictly positive definite of order $\lceil \beta \rceil + 1$.

2. *For the surface spline $\phi(r) = r^{2k}\log(r)$ the function $g(r) = r^k \log(\sqrt{r})$ is completely monotone of order $m = k+1$ and so it follows from Lemma 3.10 and Theorem 1.11 that the shifted surface spline $\phi(r) = \frac{1}{2}(r^2 + c^2)^k \log(r^2 + c^2)$ is strictly positive definite of order $m = k + 1$.*

3. *The results in the previous examples are well known but it is also possible to compute functions that have been seldom used in the context of radial basis functions. The Matern basis function*
$$\phi(r) = \frac{2^{1-\nu}}{\Gamma(\nu)}(r)^\nu K_\nu(r)$$
is strictly positive definite for arbitrary dimension d, therefore by applying Theorem 1.14 and Lemma 3.10 we conclude that the new basis function
$$\phi_c(r) = \frac{2^{1-\nu}}{\Gamma(\nu)}(\sqrt{r^2 + c^2})^\nu K_\nu(\sqrt{r^2 + c^2}) \tag{3.8}$$
is also strictly positive definite.

The described theorems are only applicable to functions that are positive definite or conditionally positive definite in arbitrary dimensions. They cannot easily be generalised to multiply monotone functions. We explicitly state here that for a multiply monotone function ϕ which is positive definite up to a certain dimension the shifted version $\phi(\sqrt{r^2 + c^2})$ is not necessarily multiply monotone or positive definite.

For multiply monotone functions a simpler form of the shift is applicable.

Lemma 3.12. *Let $\phi \in C^{k-2}((0,\infty))$ be k-time monotone on $\mathbb{R}_{>0}$ and no polynomial, then the function derived as $\tilde{\phi}_c = \phi(r+c)$ is k-times multiply monotone. Further $\tilde{\phi}_c$ is strictly positive definite on $\mathbb{R}^d$ for $k \geq \lfloor d/2 \rfloor + 2$ if $\tilde{\phi}_c$ is no polynomial.*

Proof. The lemma follows immediately from Theorem 1.24 and the definition of multiple monotonicity. □

3.2.2 Fourier transforms of shifted radial basis functions

The Fourier transform of a radial basis function is important for proving its positive definiteness, it is also necessary to determine the native space of a radial basis functions. Therefore we want to be able to derive the Fourier transform of a shifted basis function easily from the Fourier transform of the original function, where this is possible. By choosing the radial basis functions to stem from $L^1(\mathbb{R})$ we can use the Hankel transform (as defined in (1.13)) to compute their Fourier transform. For now we suppose ϕ to be a radial basis function which is positive definite in any dimension d and therefore has a Bernstein representation (as in Theorem 1.10).

Theorem 3.13. *Let $\phi \in L^1(\mathbb{R}^d)$ be a strictly positive definite radial basis function for all d. Then the d-dimensional Fourier transform of the shifted function $\phi_c(\|x\|)$ is given by*

$$\widehat{\Phi_c}(\xi) = \int_0^\infty \pi^{d/2} e^{-\|\xi\|^2/(4t)} t^{-d/2}\, d\mu_c(t). \tag{3.9}$$

Proof. Since ϕ is positive definite in arbitrary dimensions, the shift $\phi_c(r) = g(r^2+c^2)$, $r \in \mathbb{R}_{\geq 0}$, is also positive definite as proven in Theorem 3.8 and it is possible to describe $\widehat{\Phi}_c$ using the representation of (3.6):

$$\begin{aligned}\widehat{\Phi_c}(\xi) &= \frac{1}{\sqrt{2\pi}^d} \int_{\mathbb{R}^d} e^{-i\xi^t x} \phi_c(\|x\|)\, dx \\ &= \frac{1}{\sqrt{2\pi}^d} \int_{\mathbb{R}^d} \left(\int_0^\infty e^{-\|x\|^2 t}\, d\mu_c(t) \right) e^{-i\xi^T x}\, dx.\end{aligned}$$

We are now able to exchange the order of integration.

$$\begin{aligned}\widehat{\Phi_c}(\xi) &= \int_0^\infty \underbrace{\int_{\mathbb{R}^d} e^{-t^2 x} e^{-i\xi^t x}\, dx}_{\text{Fourier transform of the Gaussian}} \, d\mu_c(t) \\ &= \int_0^\infty \pi^{d/2} e^{-\|\xi\|^2/(4t)} t^{-d/2}\, d\mu_c(t).\end{aligned}$$

□

We now generalise this idea further for functions that are not positive definite in arbitrary dimensions, therefore we have to verify their positive definiteness using Bochner's Theorem (cited as Theorem 1.18). As a helpful technique we introduce a new interpretation of the shift of a radial basis function.

Considering a radial basis function $\phi : \mathbb{R}_{\geq 0}$
$rightarrow \mathbb{R}$ which is stictly positive definite on $\mathbb{R}^{d+1}$. We express the shift of this basis function as a d-dimensional radial function

$$\Phi_c(x) = \phi_c(\|x\|) = \phi(\sqrt{\|x\|^2 + c^2}) = \phi\left(\sqrt{x_1^2 + \cdots + x_n^2 + c^2}\right). \tag{3.10}$$

The last expression can be interpreted as the value of the $(d+1)$-dimensional function $\Phi(\cdot) = \phi(\|\cdot\|)$ when the last parameter is equal to c. In this section we have to dedicate special attention to the dimension used, therefore we denote elements of $\mathbb{R}^{d+1}$ with an additional $'$ as for example: x', ξ' and elements of $\mathbb{R}^d$ as before with x, ξ. According to the Bochner's theorem a radial function $\Phi(x') = \phi(\|x'\|)$ which is positive definite on $\mathbb{R}^{d+1}$ has a representation

$$\Phi(x') = (2\pi)^{-(d+1)/2} \int_{\mathbb{R}^{d+1}} e^{ix'^T\omega'}\, d\mu(\omega'),$$

where $d\mu$ is a positive Borel measure. Using the above description of $\Phi_c(x)$ in $\mathbb{R}^d$ we can see that

$$\begin{aligned}
\Phi_c(x) &= (2\pi)^{-(d+1)/2} \int_{\mathbb{R}^{d+1}} e^{ix^T(\omega_1,\ldots,\omega_d)} e^{ic\omega_{d+1}}\, d\mu(\omega') \\
&= (2\pi)^{-(d+1)/2} \int_{\mathbb{R}^d} e^{ix^T(\omega_1,\ldots,\omega_d')} \underbrace{\int_{\mathbb{R}} e^{ic\omega_{d+1}}\, d\mu(\omega')}_{=d\mu_c(\omega)}.
\end{aligned}$$

So the positive definiteness of the above depends on whether the last row introduces a positive Borel measure $d\mu_c$. This is not necessarily true, as a simple example shows: Applying the shift to a compactly supported basis function with support $[0,1]$, will result in a basis function being zero if c exceeds 1.

To be able to prove the positive definiteness of such functions we want to give a simple formula for their d-dimensional Fourier transform. For deriving this formula we make use of another observation, for functions $\Phi : \mathbb{R}^{d+1} \to \mathbb{R}$, $\Phi \in L^1(\mathbb{R}^{d+1})$, which are radial and bounded, the $(d+1)$-dimensional Fourier transform is given by

$$\widehat{\Phi}(\xi') = \frac{1}{(2\pi)^{(d+1)/2}} \int_{\mathbb{R}^{d+1}} \phi(\|x'\|) e^{-ix'^T\xi'}\, dx'.$$

We can transform this using the above definition of the shifted function, so that

$$\begin{aligned}
\widehat{\Phi}(\xi') &= \frac{1}{(2\pi)^{(d+1)/2}} \int_{\mathbb{R}} \int_{\mathbb{R}^d} \phi\left(\sqrt{\|x\|^2 + x_{d+1}^2}\right) e^{-ix^T\xi} e^{-ix_{n+1}\xi_{d+1}}\, dx\ dx_{d+1} \\
&= \frac{1}{(2\pi)^{(d+1)/2}} \int_{\mathbb{R}} e^{-ix_{d+1}\xi_{d+1}} \int_{\mathbb{R}^d} \phi_{x_{d+1}}(\|x\|) e^{-ix^T\xi}\, dx\ dx_{d+1} \\
&= \frac{1}{(2\pi)^{1/2}} \int_{\mathbb{R}} \widehat{\Phi_{x_{d+1}}}(\xi) e^{-ix_{d+1}\xi_{d+1}}\, dx_{d+1}.
\end{aligned}$$

The idea of applying the inverse Fourier transform (1.12) to the above equation motivated the following theorem which is applicable for a broader class of functions than those in $L^1(\mathbb{R}^{d+1})$.

Theorem 3.14. *Let $\Phi(x') = \phi(\|x'\|)$, $x' \in \mathbb{R}^{d+1}$, be a radial basis function, having the generalised Fourier transform $\widehat{\Phi}(\xi')$ of order k and let $x, \xi \in \mathbb{R}^d$. Then the shifted basis function $\Phi_c(x) = \phi(\sqrt{\|x\|^2 + c^2})$ has the generalised Fourier transform of order k:*

$$\widehat{\Phi_c}(\xi) = \frac{1}{(2\pi)^{1/2}} \int_{\mathbb{R}} \widehat{\Phi}(\xi') e^{-i\xi_{d+1}c}\, d\xi_{d+1} = \sqrt{\frac{2}{\pi}} \int_0^\infty \widehat{\Phi}(\xi') \cos(\xi_{d+1}c)\, d\xi_{d+1}. \qquad (3.11)$$

Proof. Since Φ has a generalised Fourier transform of order k (as defined in Definition 1.20) and is radially symmetric we know that $\Phi(x') = \mathcal{O}(\|x'\|^\ell)$ for $\|x'\| \to \infty$ and some $\ell \in \mathbb{N}$. From this it follows immediately that

$$\Phi_c(x) = \Phi(\sqrt{\|x\|^2 + c^2}) = \mathcal{O}(\|x\|^\ell), \quad \text{for } \|x\| \to \infty.$$

We now show that for $\widehat{\Phi_c}(\xi)$ as in (3.11) the equation

$$\langle \widehat{\Phi_c}, \psi \rangle = \langle \Phi_c, \widehat{\psi} \rangle$$

holds for all $\psi \in S_{2k}(\mathbb{R}^d)$. We start with the left-hand side

$$\begin{aligned}
\langle \Phi_c, \widehat{\psi} \rangle &= \int_{\mathbb{R}^d} \Phi\left((x_1, \ldots, x_d, c)^T\right) \widehat{\psi}(x)\, dx \\
&= \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}} \Phi((x_1, \ldots, x_d, x_{d+1})^T) \delta(x_{d+1} - c)\, dx_{d+1} \right) \widehat{\psi}(x)\, dx \\
&= \int_{\mathbb{R}^{d+1}} \Phi((x_1, \ldots, x_d, x_{d+1}))^T \delta(x_{d+1} - c) \widehat{\psi}(x)\, dx'.
\end{aligned}$$

Let δ_k be a Dirac sequence in $L^1(\mathbb{R})$, then we get

$$\begin{aligned}
\langle \Phi_c, \widehat{\psi} \rangle &= \int_{\mathbb{R}^{d+1}} \widehat{\psi}(x) \Phi(x') \lim_{k\to\infty} \delta_k(x_{d+1} - c)\, dx' \\
&= \lim_{k\to\infty} \int_{\mathbb{R}^{d+1}} \widehat{\psi}(x) \Phi(x') \left(\frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \left((\delta_k(\bullet - c))^\wedge (\nu) \right) e^{i\nu x_{d+1}}\, d\nu \right) dx' \\
&= \lim_{k\to\infty} \int_{\mathbb{R}^{d+1}} \widehat{\psi}(x) \Phi(x') \left(\frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{\delta}_k(\nu) e^{i\nu c} e^{i\nu x_{d+1}}\, d\nu \right) dx' \\
&= \frac{1}{\sqrt{2\pi}} \lim_{k\to\infty} \int_{\mathbb{R}^{d+1}} \int_{\mathbb{R}} \underbrace{\widehat{\psi}(x) e^{-i\nu x_{d+1}} \hat{\delta}_k(\nu)}_{=\tilde{\psi}(x')} \Phi(x') e^{i\nu c}\, d\nu\ dx' \\
&= \frac{1}{\sqrt{2\pi}} \lim_{k\to\infty} \int_{\mathbb{R}} \int_{\mathbb{R}^{d+1}} \underbrace{\widehat{\psi}(x) e^{-i\nu x_{d+1}} \hat{\delta}_k(\nu)}_{=\tilde{\psi}(x')} \Phi(x')\, dx' e^{i\nu c}\, d\nu.
\end{aligned}$$

We are allowed to exchange limits in the above equation because of the decay and asymptotic properties of $\Phi(x')$ and $\widehat{\psi}$. Since the generalised Fourier transform of Φ' is known,

$$(\psi(\xi)\delta_k(\nu - \xi_{d+1}))^\wedge (x') = \tilde{\psi}(x'),$$

and $\psi(\xi)\delta_k(\nu - \xi_{d+1}) \in S_{2k}(\mathbb{R}^{d+1})$ as a function of ξ'. We conclude

$$\begin{aligned}
\langle \Phi_c, \widehat{\psi} \rangle &= \lim_{k\to\infty} \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_{\mathbb{R}^{d+1}} \psi(\xi) \delta_k(\nu - \xi_{d+1}) \widehat{\Phi}((\xi_1, \ldots, \xi_d, \xi_{d+1}))^T\, d\xi'\, e^{i\nu c}\, d\nu \\
&= \int_{\mathbb{R}^d} \psi(\xi) \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \lim_{k\to\infty} \int_{\mathbb{R}} \delta_k(\nu - \xi_{d+1}) \widehat{\Phi}((\xi_1, \ldots, \xi_{d+1}))^T\, d\xi_{d+1} e^{i\nu c}\, d\nu\ d\xi \\
&= \int_{\mathbb{R}^d} \psi(\xi) \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \widehat{\Phi}((\xi_1, \ldots, \xi_d, \nu))^T e^{i\nu c}\, d\nu\ d\xi \\
&= \langle \widehat{\Phi_c}, \psi \rangle.
\end{aligned}$$

The last equation holds, because $\widehat{\Phi}$ is symmetric in ξ_{d+1}. $\square$

Example 3.15. *As a first example for the application of this theorem, we compute the*

Fourier transform of the multiquadric. The multiquadric is, for now, be regarded as shift of the basis function $\phi(\|x'\|) = \|x'\|^{2\beta}$, for $\beta \in \mathbb{R}_{>0} \setminus \mathbb{N}$, (see [Wen05]), its generalised Fourier transform of order $k = 2\beta$ in $\mathbb{R}^{d+1}$ is

$$\widehat{\Phi}(\xi') = \frac{2^{2\beta+\frac{d+1}{2}}}{\Gamma(-\beta)}\Gamma((d+1+2\beta)/2) \cdot \|\xi'\|^{-2\beta-d-1}. \tag{3.12}$$

Applying Theorem 3.14, we get:

$$\begin{aligned}\widehat{\Phi_c}(\xi) &= \sqrt{\frac{2}{\pi}} \int_0^\infty \hat{\Phi}(\xi') \cos(\xi_{d+1}c)\, d\xi_{d+1} \\ &= \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{2^{2\beta+\frac{d+1}{2}}}{\Gamma(-\beta)}\Gamma\left((d+1+2\beta)/2\right) \cdot \|\xi'\|^{-2\beta-d-1} \cos(\xi_{d+1}c)\, d\xi_{d+1} \\ &= \sqrt{\frac{2}{\pi}} \frac{2^{2\beta+\frac{d+1}{2}}}{\Gamma(-\beta)}\Gamma\left((d+1+2\beta)/2\right) \int_0^\infty \frac{1}{(\|\xi\|^2+\xi_{d+1}^2)^{+\beta+(d+1)/2}} \cos(\xi_{d+1}c)\, d\xi_{d+1}.\end{aligned}$$

The integral can be transformed into the modified Bessel function ([AS72] 9.6.25) given as in Equation (1.1). *We therefore conclude*

$$\begin{aligned}\widehat{\Phi_c}(\xi) &= \sqrt{\frac{2}{\pi}} \frac{2^{2\beta+\frac{d+1}{2}}}{\Gamma(-\beta)} K_{\frac{d}{2}+\beta}(c\|\xi\|) 2^{-(\frac{d}{2}+\beta)} \cdot \left(\frac{c}{\|\xi\|}\right)^{\frac{d}{2}+\beta} \pi^{\frac{1}{2}} \\ &= \frac{2^{\beta+1}}{\Gamma(-\beta)} \left(\frac{\|\xi\|}{c}\right)^{-\beta-\frac{d}{2}} K_{\frac{d}{2}+\beta}(c\|\xi\|).\end{aligned}$$

Remark 3.16. *In a way similar to the previous example we can compute the shift of a basis function $\phi(x) = \|x\|^\beta$ with $\beta < 0$, normally we use the shift parameter c to smooth the function, but in this case it eliminates the singularity the functions has in zero. An important special case of $\beta < 0$ is the one where $c = 1$. In this case we can apply the relation $K_\nu(x) = K_{-\nu}(x)$ and observe that the Matérn kernel*

$$\widehat{\Phi}(\xi) = \|\xi\|^\upsilon K_\upsilon(\xi), \quad \upsilon \geq 0,$$

is the Fourier transform of the inverse multiquadric

$$\phi(x) = \frac{1}{(1+x^2)^\gamma}, \quad \gamma = \upsilon + \frac{d}{2} \in \mathbb{R}_{>0} \setminus \mathbb{N}, \quad \gamma > d/2.$$

Example 3.17. *We are also able to compute the Fourier transform of the shifted thin-plate spline by applying the new theorem. The method is the same as in the last example, but*

$$\phi(\|x'\|) = \|x'\|^{2k} \log(\|x'\|), \quad k \in \mathbb{N}_{>0},$$

its Fourier transform of order $k+1$ is taken from [Wen05] Theorem 8.17:

$$\widehat{\Phi}(\xi') = (-1)^{k+1} 2^{2k-1+d/2} \Gamma(k + d/2) k! \|\xi'\|^{-d-2k}.$$

By applying (3.11) *we can easily derive that for the shifted version*

$$\Phi_c(x) = (\|x\|^2 + c^2)^k \log(\|x\|^2 + c^2)^{\frac{1}{2}}, \quad k \in \mathbb{N}_{>0},$$

the generalised d-dimensional Fourier transform of order $k+1$ is

$$\widehat{\Phi_c}(\xi) = 2^k (-1)^{k+1} \left(\frac{c}{\|\xi\|}\right)^{d/2+k} K_{\frac{d}{2}+k}(c\|\xi\|). \tag{3.13}$$

As was the case for the multiquadric, the shifted thin-plate spline is well known, as are their Fourier transforms. So we now compute the Fourier transform of a radial basis function which, to our knowledge, has not been considered before.

Example 3.18. *For the Matérn basis function we can deduce from Equation* (1.1) *that*

$$\phi(\|x'\|) = \frac{2^{1-\nu}}{\Gamma(\nu)} \|x'\|^{\nu} K_{\nu}(\|x'\|) = \int_0^{\infty} \frac{\cos(\|x'\|t)}{(t^2+1)^{\nu+\frac{1}{2}}}\, dt$$

which shows that the Fourier transform for $\xi' \in \mathbb{R}^{d+1}$ is given by

$$\hat{\Phi}(\xi') = (1 + \|\xi'\|^2)^{-\nu-\frac{d+1}{2}}.$$

We now apply Theorem 3.14 to find the Fourier transform of the shifted Matérn kernel

$$\phi_c(\|x\|) = \frac{2^{1-\nu}}{\Gamma(\nu)} K_{\nu}\left(\sqrt{\|x\|^2 + c^2}\right) \left(\|x\|^2 + c^2\right)^{\nu/2},$$

for $\nu > 0$ and $2\nu \notin \mathbb{N}$ (otherwise the function $\phi(\|x'\|)$ reduces to the product of a polyno-

mial and an exponential). The Fourier transform is

$$\begin{aligned}\widehat{\Phi}_c(\xi) &= \sqrt{\frac{2}{\pi}}\int_0^\infty (1+\|\xi\|^2+\xi_{d+1}^2)^{-\nu-\frac{d+1}{2}}\cos(c\xi_{d+1})\,d\xi_{d+1}\\ &= \sqrt{\frac{2}{\pi}}\int_0^\infty \left((\sqrt{1^2+\|\xi\|^2})^2+\xi_{d+1}^2\right)^{-\nu-\frac{d+1}{2}}\cos(c\xi_{d+1})\,d\xi_{d+1}.\end{aligned}$$

Using [GR14] (3.771.2) we can further deduce

$$\begin{aligned}\widehat{\Phi}_c(\xi) = \frac{\sqrt{2}}{\pi}\cos\left(\pi\left(-\nu-\frac{d}{2}\right)\right)\Gamma\left(-\nu-\frac{d-1}{2}\right)\\ \cdot\left(\frac{2\sqrt{1+\|\xi\|^2}}{c}\right)^{-\nu-\frac{d}{2}} K_{-\nu-\frac{d}{2}}\left(c\sqrt{1+\|\xi\|^2}\right).\end{aligned} \tag{3.14}$$

This function is positive for all $\nu > 0$ *because the* $\cos\left(\pi(-\nu-\frac{d}{2})\right)$ *and the gamma function* $\Gamma\left(-\nu-\frac{d-1}{2}\right)$ *have the same sign for any* ν.

In the previous section we were able to deduce simple conditions for positive definiteness of functions possessing certain monotonicity properties, if the function to be shifted does not possess such properties, we can only deduce the positive definiteness using Theorem 1.18 or conditionally positive definiteness using Definition 1.20.

Lemma 3.19. *Let* ϕ *be a conditionally positive definite function of order* k *on* $\mathbb{R}^{d+1}$. *Then* $\Phi_c(\|x\|) = \phi(\sqrt{\|x\|^2+c^2})$ *is a radial basis function, which is conditionally positive definite of order* k *in* $\mathbb{R}^d$ *if*

$$\widehat{\Phi}_{d+1}(\|\xi'\|) = \|\xi'\|^{-\frac{d-1}{2}}\int_0^\infty \phi(t)t^{\frac{d+1}{2}}J_{\frac{d-2}{2}}(\|\xi'\|t)\,dt$$

is the $(d+1)$*-dimensional generalised Fourier transform of* ϕ *and*

$$h(t) = \int_0^\infty \widehat{\Phi}_{d+1}(\sqrt{t^2+\tilde{c}^2})e^{-i\tilde{c}c}\,d\tilde{c} > 0, \quad \forall t \geq 0. \tag{3.15}$$

Proof. Follows directly from the integral representation in Equation (3.11). □

3.3 The inverse Gaussian class of radial basis functions

In this section we make use of Bochner's theorem (cited as Theorem 1.18) to construct a new class of radial basis functions. The technique has already been described and used for other functions but the set of radial basis functions, which includes the inverse multiquadric and the Gaussian as a special case has not been considered before.

By computing the Fourier transform of a function $\Psi(x) \in L^1(\mathbb{R}^d)$ which is positive on $\mathbb{R}^d$ and not constant, we can identify $\widehat{\Psi}$, if it is in $L^1(\mathbb{R}^d)$, as a new positive definite basis function on $\mathbb{R}^d$. If Ψ is a radial function, then $\widehat{\Psi} = \Phi$ will be a positive definite radial basis function. Thereby every completely or multiply monotone function describe in the previous chapters can be used to derive new positive definite basis functions, which themselves will not necessarily posses any monotonicity properties.

The examples given in the previous section can also be used as examples for the described idea. The Matern kernel (Example 3.18) is the d-dimensional Fourier transform of an inverse multiquadric for $\beta \notin \mathbb{Z}$. The inverse multiquadric is positive on $\mathbb{R}^d$ and integrable, so the Matern kernel is positive definite. Considering the various examples in the last section we see that the Fourier transforms of the class $\|\cdot\|^\beta$ are well studied for $\beta \in \mathbb{R}$. We now want to investigate the class of Fourier transforms of the functions

$$\Psi(\|x\|) = e^{-\|x\|^\beta}, \tag{3.16}$$

which are integrable for $\beta > 0$ and positive, so that the d-dimensional Fourier transforms of those functions will exists and be positive definite on $\mathbb{R}^d$. We start by gathering informations about the special choices of β which are already known and used as radial basis functions.

Example 3.20. • $\beta = 1$*: In this case the function is*

$$\Psi(x) = e^{-\|x\|},$$

which is the Poisson kernel. Its Fourier transform is

$$\widehat{\Psi}(\xi) = 2^{d/2-1/2}\Gamma\left(\frac{d}{2}+\frac{1}{2}\right)\frac{1}{(1+\|\xi\|^2)^{\frac{d}{2}+\frac{1}{2}}},$$

which is a special case of the generalised inverse multiquadric, $\phi(r) = (1+r^2)^{\alpha/2}$*, with* $\alpha = -d-1$ *(displayed in Figure 3.1),*

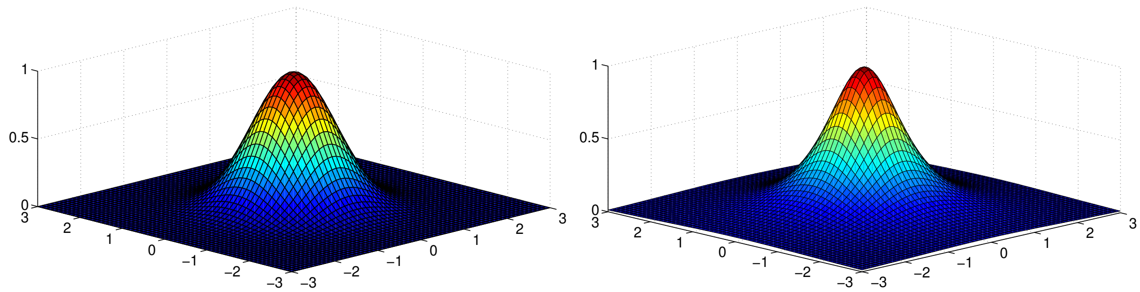

Figure 3.1: The Gaussian in two dimensions $\beta = 2$, the Fourier transform of $e^{-\|x\|}$ ($\beta = 1$)

- *$\beta = 2$: The function is the Gaussian basis function $\Psi(x) = e^{-\|x\|^2}$, which has the Fourier transform $\widehat{\Psi}(\xi) = (1/2)^{d/2} e^{-\|\xi\|^2/4}$ which is also a Gaussian basis function (displayed in Figure 3.1),*

- *$\beta = 2n$: The function is $\Psi(x) = e^{-\|x\|^{2n}}$ its Fourier transform was considered, for the case $d = 1$ in [Boy14]. The Fourier transforms of $\psi(x) = e^{|x|^{A2n}}$ have therein been approximated without giving a representation different from the obvious integral description. For the special case $\beta = 4$ the resulting radial basis function is called the inverse quartic Gaussian ($\beta = 4$, Figure 3.2). A series representation has been computed using Matlab by Boyd in [BM13] and takes the form*

$$\widehat{\Psi}(\xi) = \frac{\sqrt{\pi}}{2} \sum_{k=0}^{\infty} \frac{\Gamma(1/2)}{\Gamma(1/2+n)\Gamma(3/4+k)} \frac{\left(\frac{|\xi|}{4}\right)^{4k}}{k!}$$
$$- \frac{1}{4\sqrt{2\pi}} \Gamma(3/4)|\xi|^2 \sum_{k=0}^{\infty} \frac{\Gamma(5/4)\Gamma(3/2)}{\Gamma(3/2+k)\Gamma(5/4+k)} \frac{\left(\frac{|\xi|}{4}\right)^{4k}}{k!}. \quad (3.17)$$

We now give a representations of the d-dimensional Fourier transform of $\Psi(x) = e^{-\|x\|^{\beta}}$. We focus on the case $\beta \geq 1$ using the series representation of the Bessel function already introduced in (1.14). However to be able to compute the Fourier transform we need to prove this additional lemma first.

Lemma 3.21. *The series*

$$\sum_{k=0}^{\infty} (-1) a^{2k} \frac{\Gamma\left(\frac{d+2k}{\beta}\right)}{\Gamma(k+1)\Gamma(k+\frac{d}{2})}, \quad a \in \mathbb{R}, \quad (3.18)$$

is absolutely convergent for every $\beta > 1$.

Proof. We can estimate the Gamma function using Stirling's formula ([GR14], (8.327.1)) and deduce

$$\Gamma\left(\frac{d+2k}{\beta}\right) \leq \left(\frac{d+2k}{\beta}\right)^{\frac{d+2k}{\beta}-\frac{1}{2}} e^{-\frac{d+2k}{\beta}} \left(1+\frac{1}{6}\left(\frac{\beta}{d+2k}\right)\right)\sqrt{2\pi}$$
$$\leq \left(\frac{d+2k}{\beta}\right)^{\frac{d+2k}{\beta}-\frac{1}{2}} e^{-\frac{d+2k}{\beta}} 2^{\frac{3}{2}}\sqrt{\pi},$$

for sufficiently large k. Using the same formula we derive a lower bound

$$\Gamma(k+1) \geq (k+1)^{k+1-\frac{1}{2}} e^{-(k+1)}\sqrt{2\pi},$$
$$\Gamma\left(k+\frac{d}{2}\right) \geq \left(k+\frac{d}{2}\right)^{k+\frac{d}{2}-\frac{1}{2}} e^{-\left(k+\frac{d}{2}\right)}\sqrt{2\pi}.$$

Therefore we can determine an estimate of the coefficients of the series for fixed values of d, $\beta > 0$. Here $C \in \mathbb{R}_{>0}$, $\alpha \in \mathbb{R}$, $\gamma \in \mathbb{R}_{>0}$, are parameters that can represent a different value in every use,

$$\left| a^{2k} \frac{\Gamma\left(\frac{d+2k}{\beta}\right)}{\Gamma(k+1)\Gamma(k+\frac{d}{2})} \right| \leq |a^{2k}| \frac{2(\frac{d+2k}{\beta})^{\frac{d+2k}{\beta}-\frac{1}{2}} e^{-\frac{d+2k}{\beta}}}{\sqrt{2\pi}(k+1)^{k+\frac{1}{2}} e^{-(k+1)}(k+\frac{d}{2})^{k+\frac{d}{2}-\frac{1}{2}} e^{-\left(k+\frac{d}{2}\right)}}$$
$$\leq C|a^{2k}| e^{-\frac{2k}{\beta}+2k} \beta^{-\frac{2k}{\beta}} \frac{(d+2k)^{\frac{d+2k}{\beta}-\frac{1}{2}}}{(k+1)^{k+\frac{1}{2}}(k+\frac{d}{2})^{k+\frac{d}{2}-\frac{1}{2}}}$$
$$\leq C\gamma^{2k} e^{\alpha k}(k+1)^{-0.5}\left(k+\frac{d}{2}\right)^{-\frac{d}{2}} \frac{(d+2k)^{\frac{d+2k}{\beta}}}{(k+1)^k(k+\frac{d}{2})^k}.$$

We take $d \geq 2$, for the case $d = 1$ works analogously,

$$\left| a^{2k} \frac{\Gamma\left(\frac{d+2k}{\beta}\right)}{\Gamma(k+1)\Gamma(k+\frac{d}{2})} \right| \leq C\gamma^{2k} e^{\alpha k}(k+1)^{-0.5}\left(k+\frac{d}{2}\right)^{-\frac{d}{2}} (d+2k)^{\frac{d}{\beta}} \frac{(d(1+\frac{2}{d}k))^{\frac{2k}{\beta}}}{(k+1)^{2k}}$$
$$\leq C\gamma^{2k} e^{\alpha k}(k+1)^{-0.5}(d+2k)^{\frac{d}{\beta}-\frac{d}{2}}(1+k)^{\frac{2k}{\beta}-2k}$$
$$\leq \mathcal{O}\left(k^{\frac{2k}{\beta}-2k}\right),$$

which gives a convergent series for $\frac{2k}{\beta} - 2k < 0$ which is true for all $\beta > 1$. □

Lemma 3.22. *The Fourier transform of* $\Psi(x) = e^{-\|x\|^\beta}$, $x \in \mathbb{R}^d$, $\beta > 1$ *is*

$$\widehat{\Psi}(\xi) = 2^{-\frac{d}{2}+1}\frac{1}{\beta}\sum_{k=0}^{\infty} \frac{(-1)^k \left(\frac{\|\xi\|}{2}\right)^{2k}}{k!\Gamma(k+\frac{d}{2})}\Gamma\left(\frac{d+2k}{\beta}\right). \tag{3.19}$$

Proof. We use Theorem 1.17 to compute the Fourier transform; this is applicable because $\Psi \in L^1(\mathbb{R}^d)$, for all $\beta > 1$, and $d \in \mathbb{N}$. We then use the series representation of the Bessel function ([AS72] (9.1.10))

$$\begin{aligned}
\widehat{\Psi}(\xi) &= \|\xi\|^{-(\frac{d-2}{2})} \int_0^\infty e^{-t^\beta} t^{d/2} J_{\frac{d-2}{2}}(\|\xi\| t)\, dt \\
&= \|\xi\|^{-(\frac{d-2}{2})} \int_0^\infty e^{-t^\beta} t^{d/2} \sum_{k=0}^\infty \frac{(-1)^k (\|\xi\| t/2)^{2k+\frac{d}{2}-1}}{k!\Gamma(k+\frac{d}{2})}\, dt \\
&= 2^{-\frac{d}{2}+1} \int_0^\infty e^{-t^\beta} t^{d-1} \sum_{k=0}^\infty \frac{(-1)^k \left(\frac{\|\xi\| t}{2}\right)^{2k}}{k!\Gamma(k+\frac{d}{2})}\, dt \\
&= 2^{-\frac{d}{2}+1} \lim_{u\to\infty} \int_0^u e^{-t^\beta} t^{d-1} \lim_{n\to\infty} \sum_{k=0}^n \frac{(-1)^k \left(\frac{\|\xi\| t}{2}\right)^{2k}}{k!\Gamma(k+\frac{d}{2})}\, dt.
\end{aligned}$$

We can exchange the order of the limits because

$$\left| \sum_{k=0}^n \frac{(-1)^k \left(\frac{\|\xi\| t}{2}\right)^{2k}}{k!\Gamma(k+\frac{d}{2})} \right| \le \sum_{k=0}^\infty \left| \frac{\left(\frac{\|\xi\| t}{2}\right)^{2k}}{k!\Gamma(k+\frac{d}{2})} \right| \le e^{\frac{1}{4}(\|\xi\| t)^2} + a, \quad a \in \mathbb{R},$$

with $\frac{1}{\Gamma(k+d/2)} < 1$, for $k > 2$, which gives an integrable majorant on $[0, u]$. Thereby we get

$$\begin{aligned}
\widehat{\Psi}(\xi) &= 2^{-\frac{d}{2}+1} \lim_{u\to\infty} \sum_{k=0}^\infty \frac{(-1)^k \left(\frac{\|\xi\|}{2}\right)^{2k}}{k!\Gamma\left(k+\frac{d}{2}\right)} \int_0^u e^{-t^\beta} t^{d-1+2k}\, dt \\
&= 2^{-\frac{d}{2}+1} \lim_{u\to\infty} \sum_{k=0}^\infty \frac{(-1)^k \left(\frac{\|\xi\|}{2}\right)^{2k}}{k!\Gamma(k+\frac{d}{2})} \int_0^{u^\beta} e^{-z} z^{\frac{d+2k}{\beta}-1} \frac{1}{\beta}\, dz \\
&\overset{(3.381.1)[\text{GR14}]}{=} 2^{-\frac{d}{2}+1} \frac{1}{\beta} \lim_{u\to\infty} \sum_{k=0}^\infty \frac{(-1)^k \left(\frac{\|\xi\|}{2}\right)^{2k}}{k!\Gamma\left(k+\frac{d}{2}\right)} \gamma\left(\frac{d+2k}{\beta}, u^\beta\right).
\end{aligned}$$

Here $\gamma(\cdot,\cdot)$ is the incomplete Γ-function. We know that $\gamma\left(\frac{d+2}{k}, u^\beta\right) \le \Gamma\left(\frac{d+2k}{\beta}\right)$ for all $\beta > 1$ and applying Lemma 3.21 we get a convergent majorant. The definition of the incomplete gamma function then gives

$$\widehat{\Psi}(\xi) = 2^{-\frac{d}{2}+1}\frac{1}{\beta}\sum_{k=0}^{\infty}\frac{(-1)^k\left(\frac{\|\xi\|}{2}\right)^{2k}}{k!\Gamma\left(k+\frac{d}{2}\right)}\Gamma\left(\frac{d+2k}{\beta}\right).$$

□

Theorem 3.23. *The function*

$$\psi(r) = 2^{-\frac{m}{2}+1}\frac{1}{\beta}\sum_{k=0}^{\infty}\frac{(-1)^k\left(\frac{r}{2}\right)^{2k}}{k!\Gamma(k+\frac{m}{2})}\Gamma\left(\frac{m+2k}{\beta}\right) \tag{3.20}$$

is as a strictly positive definite radial function on $\mathbb{R}^d$ *if* $m \geq d$ *and* $\beta > 1$.

Proof. The theorem follows immediately from Lemma 3.22 together with Theorem 1.21 because

$$\psi(x) = \int_{\mathbb{R}^m} e^{-\|y\|^\beta} e^{ix^Ty} dy \tag{3.21}$$

under the given conditions on d and β, and because $e^{-\|x\|^\beta} > 0$ and is integrable for all $\beta > 0$. □

The last series is absolute convergent for $\beta > 1$ and can be further simplified for many values of β by applying the doubling or tripling formulas for the Gamma function. We illustrate this by determining a multivariate generalisation of the inverse quartic Gaussian, described by Boyd in [BM13] and [Boy14] for $d = 1$. This includes the calculation of the formula of Boyd which they derived using Maple, as a special case.

Example 3.24. *We take* $\beta = 4$ *then for the so called inverse quartic Gaussian in dimension* d *which is the Fourier transform of* $\Psi(x) = e^{-\|x\|^4}$, $x \in \mathbb{R}^d$, *we find the representation*

$$\begin{aligned}\widehat{\Psi}(\xi) &= 2^{-\frac{d}{2}-1}\sum_{k=0}^{\infty}\frac{(-1)^k\left(\frac{\|\xi\|}{2}\right)^{2k}}{k!\Gamma(k+\frac{d}{2})}\Gamma\left(\frac{d+2k}{4}\right)\\ &= 2^{-d/2-1}\left(\sum_{k=0}^{\infty}\frac{\left(\frac{\|\xi\|}{2}\right)^{4k}\Gamma(\frac{d}{4}+k)}{\Gamma(2k+1)\Gamma(2k+\frac{d}{2})} - \left(\frac{\|\xi\|}{2}\right)^2\sum_{k=0}^{\infty}\frac{\left(\frac{\|\xi\|}{2}\right)^{4k}\Gamma(\frac{d+2}{4}+k)}{\Gamma(2k+2)\Gamma(2k+1+\frac{d}{2})}\right).\end{aligned} \tag{3.22}$$

Now we apply the doubling formula for the Gamma function

$$\Gamma(2z) = (2\pi)^{-1/2}\, 2^{2z-1/2}\Gamma(z)\Gamma\left(z+\frac{1}{2}\right)$$

from [AS72] (6.1.18) to $\Gamma(2k+1)$, $\Gamma(2k+d/2)$, $\Gamma(2k+2)$ *and* $\Gamma(2k+1+d/2)$. *This gives us*

$$\begin{aligned}
\widehat{\Psi}(\xi) =& \frac{\pi}{2^d}\left(\sum_{k=0}^{\infty}\frac{\left(\frac{\|\xi\|}{4}\right)^{4k}\Gamma(\frac{d}{4}+k)}{\Gamma(k+1/2)\Gamma(k+1)\Gamma(d/4+k)\Gamma(d/4+k+1/2)}\right.\\
&\left.-\left(\frac{\|\xi\|}{2}\right)^2 2^{-2}\sum_{k=0}^{\infty}\frac{\left(\frac{\|\xi\|}{4}\right)^{4k}\Gamma(\frac{d+2}{4}+k)}{\Gamma(k+1)\Gamma(k+3/2)\Gamma(d/4+k+1/2)\Gamma(d/4+k+1)}\right)\\
=&\frac{\pi}{2^{d+4}}\left(16\sum_{k=0}^{\infty}\frac{\left(\frac{\|\xi\|}{4}\right)^{4k}}{k!\Gamma(k+1/2)\Gamma(d/4+k+1/2)}\right.\\
&\left.-\|\xi\|^2\sum_{k=0}^{\infty}\frac{\left(\frac{\|\xi\|}{4}\right)^{4k}}{k!\Gamma(k+3/2)\Gamma(d/4+k+1)}\right)\\
=&\frac{\sqrt{\pi}}{2^{d+4}}\left(\frac{16}{\Gamma(\frac{3}{4})}F\left(\{\};\frac{1}{2},\frac{d}{4}+\frac{1}{2},\left(\frac{\|\xi\|}{4}\right)^4\right)-\frac{2\|\xi\|^2}{\Gamma(\frac{5}{4})}F\left(\{\};\frac{3}{2},\frac{d}{4}+1,\left(\frac{\|\xi\|}{4}\right)^4\right)\right).
\end{aligned}$$

Setting $d=1$ *in the above gives the representation of the inverse Gaussian by Boyd (cited as* (3.17)*).*

Figure 3.2 shows that for $d=1$ the inverse quartic Gaussian ($\beta=4$) is an oscillatory radial basis function. For a long time the research on radial basis functions focused only on positive radial basis functions because, as already mentioned, only positive functions can be positive definite in arbitrary dimensions. Later compactly supported radial basis functions were studied and only in the last few years oscillatory radial basis functions were described and tested (see for example [FLW06], [BM13]). We want to find out for which values of β the described generalised inverse Gaussian is positive. One way to determine the positivity is to check whether the Fourier transform is positive definite. We know that the Fourier transform of our function is $\Psi(t)=e^{-\|x\|^\beta}$, $x\in\mathbb{R}^d$. Therefore we first check for which values of β, $g(t)=e^{-t^{\beta/2}}$ is completely monotone, which as described in Theorem 1.14 indicates positive definiteness.

Lemma 3.25. *The function* $e^{-t^{\beta/2}}$ *is completely monotone if and only if* $0\le\beta\le2$.

Proof. For $0\le\beta<2$ the complete monotonicity follows from the results in chapter 2, specifically Theorem 2.3, because $t^{\beta/2}$ possess a derivative which is completely monotone

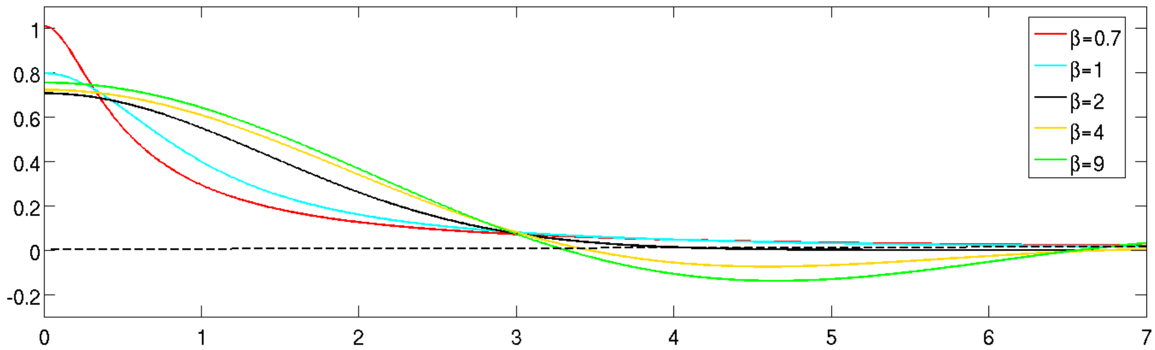

Figure 3.2: Form of the inverse Gaussian for different values of β and $d = 1$

and e^{-t} is completely monotone. For $\beta > 2$ the second derivative of $f(t) = e^{-t^{\beta/2}}$ is

$$f''(t) = e^{-t^{\beta/2}} t^{\beta/2-2} \left(\frac{\beta}{2} \left(t^{\beta/2} \frac{\beta}{2} + 1 \right) - \frac{\beta^2}{4} \right)$$

which is negative for all t satisfying $0 < t < \left(1 - \frac{2}{\beta}\right)^{2/\beta}$. We also note that for $\beta < 0$ it is not completely monotone. □

Lemma 3.26. *The function ψ defined in* (3.20) *satisfies*

$$\psi(r) > 0, \ \forall r \in [0, \infty),$$

if $0 < \beta \leq 2$.

Proof. The statement follows because Lemma 3.25 shows that e^{-t^β} is positive definite for arbitrary d if $0 < \beta \leq 2$. From (3.21) and Bochner's theorem we deduce that φ is positive as a Fourier transform of a positive definite function. □

Finally, we end this chapter by giving some examples of the shape of the newly derived basis functions. In Figure 3.2 we display the inverse Gaussian in one dimension for several different values of $\beta > 0$. As shown in the above lemma the inverse Gaussian is a positive function for $0 \leq \beta \leq 2$ and we can see the zeros of the function for $\beta = 4$ and $\beta = 9$.

Chapter 4

Interpolation on the unit sphere

Accurate and easily implementable interpolation techniques on spheres are in high demand. Especially due to their applicability in geoscience when the data is collected on the surface of the earth. The increased interest in this topic might therefore be a result of the new technologies like satellites, which make global data accessible to researchers of many disciplines, and increased computational power, which allows the researchers to efficiently process the data. A different interesting application is described in [JKBS16], where the 2-sphere is used in physiologies as a simple model of the human head.

It is of course possible to use the interpolation described in the previous chapters to derive interpolants from data situated on a unit sphere which we define as

$$\mathbb{S}^{d-1} := \{x \in \mathbb{R}^d \ : \ \|x\|_2 = 1\}.$$

The previous chapter imposed no conditions on the distribution of the data in $\mathbb{R}^d$ and the $(d-1)$-dimensional sphere is embedded in $\mathbb{R}^d$. The approach seems to work sufficiently well in some contexts but there are at least three reasons to study the interpolation on spheres more closely.

The first reason is that when using radial basis functions the influence of the measurement at one data point to an evaluation point is mainly depending on the Euclidean distance between the two points. If the data which should be interpolated is stemming from, for example, temperature measurements on the earth's surface, we would think of the geodesic distance as a more accurate tool to describe the influence a measured temperature value at one data site has on the temperature at another point. The geodesic distance measures the distance between two points, as length of the shortest arcs of a great circle connecting both points. An example of the geodesic distance on the 2-sphere is displayed in Figure 4.1. On the general unit sphere the geodesic can be measured using

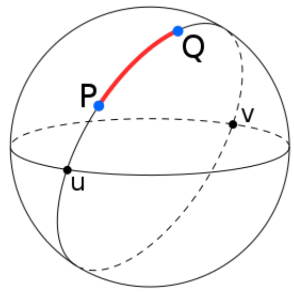

Figure 4.1: The geodesic distance

Source: https://commons.wikimedia.org/wiki/File:Illustration_of_great-circle_distance.svg(24.08.18)

the formula

$$d(\xi, \zeta) = \arccos(\xi^T \zeta), \tag{4.1}$$

if $\xi, \zeta \in \mathbb{R}^d$ are represented in Euclidean coordinates.

The second reason for developing a theory for spherical interpolation is that most of the error estimates existing for radial basis functions in $\mathbb{R}^d$ are not applicable if the data is only distributed on the sphere. For example many of the results presented in [Wen05] for Euclidean basis functions require the mesh norm of the data set

$$h_{\Xi,\Omega} = \sup_{x \in \Omega} \min_{\xi \in \Xi} \|x - \xi\|, \tag{4.2}$$

where $\Omega \subset \mathbb{R}^d$ is open, to become increasingly small. Other results like the ones described by Buhmann [Buh03] require the interpolation on an infinite grid. Johnson in [Joh98] derived estimates for interpolation with thin-plate splines and data distributed in the unit ball, but still the results did not apply if all data sites are on the unit sphere.

The third reason is that even though we can use all of the basis functions described in the previous chapters, we will demonstrate that the class of positive definite functions on the sphere $\mathbb{S}^{d-1}$ is much bigger than those. In fact, the results of Section 4.2 show that restricting attention to only positive definite functions already used in the Euclidean space leaves out the majority of the positive definite spherical functions.

In the following section we introduce the necessary notations and review some recent error estimates for the interpolation.

4.1 Introduction II

In this section we collect the notation that is used throughout the rest of the chapter and introduce the necessary tools to prove results about spherical radial basis function. We start with the definition of spherical harmonics. Spherical harmonics can be regarded as an analogue of the polynomials in $\mathbb{R}^d$ and are therefore very important for our further studies.

Definition 4.1. *Let p be a polynomial in d variables of total degree k, p is called* homogeneous *if $p(\lambda x) = \lambda^k p(x)$. The polynomial is said to be* harmonic *if $\triangle_d p = 0$ where $\triangle_d := \sum_{i=1}^d \frac{\partial^2}{\partial x_i^2}$. A* spherical harmonic of degree k, *is the restriction of a harmonic homogeneous polynomial of degree k to the sphere $\mathbb{S}^{d-1}$.*

We denote the space of all spherical harmonics of degree k on the sphere $\mathbb{S}^{d-1}$ by $H_k^*(\mathbb{S}^{d-1})$. One important property of spherical harmonics is that they are the eigenfunctions of the Laplace-Beltrami operator on the sphere. The Laplace-Beltrami operator $\triangle_{d-1}^*$ can be derived from the Laplace operator $\triangle_d$ by

$$\triangle_{d-1}^* f = \triangle_d f\left(\frac{x}{\|x\|}\right).$$

A connection is derived by replacing $x \in \mathbb{R}^d$ with $x = r\xi$ where $r = \|x\|_2$ and $\xi \in \mathbb{S}^{d-1}$, then

$$\triangle_d = \frac{\partial^2}{\partial r^2} + \frac{d-1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\triangle_{d-1}^*. \tag{4.3}$$

From the properties of being harmonic and homogeneous and the last equation it follows directly that the spherical harmonics satisfy

$$\triangle_{d-1}^* Y_k = (k(k+d-2))Y_k, \quad \text{for all } Y_k \in H_k^*(\mathbb{S}^{d-1}),$$

meaning that $H_k^*(\mathbb{S}^{d-1})$ is the eigenspace corresponding to the eigenvalue $\lambda_k = k(k+d-2)$. This is especially important for the connection to interpolation on general Riemannian manifolds, as described in [DNW97]. The dimension of $H_k^*(\mathbb{S}^{d-1})$ is the same as the multiplicity of the eigenvalue λ_k. Those are given by

$$N_{0,d} = 1 \text{ and } N_{d,k} = \frac{2k+d-2}{k}\binom{k+d-3}{k-1}, \quad k \geq 1. \tag{4.4}$$

Consequently it is possible to choose an orthonormal basis, consisting of spherical harmonics

$$Y_{j,\ell}, \quad j = 0, \ldots, k, \text{ and } \ell = 0, \ldots, N_{d,k},$$

for the space of spherical harmonics of degree at most k,

$$H_k^+(\mathbb{S}^{d-1}) = \bigoplus_{j=0}^{k} H_j^*(\mathbb{S}^{d-1}).$$

There are different possible choices of this orthonormal basis and the notation differs in the literature, that is why we are not settling with one explicit basis at the moment. There are several good books and papers on this topics including [Mue66] which we recommend for further information. From there we also take some important features of spherical harmonics. Spherical harmonics of different degree are orthogonal with respect to

$$\langle f, g\rangle_{\mathbb{S}^{d-1}} = \int_{\mathbb{S}^{d-1}} f(x)g(x)\, d\omega_{\mathbb{S}^{d-1}},$$

where $d\omega_{\mathbb{S}^{d-1}}$ is the surface area measure on the sphere $\mathbb{S}^{d-1}$ and $\omega_d = \int_{\mathbb{S}^{d-1}} d\omega_{\mathbb{S}^{d-1}} = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ is the surface area. Since the following equality holds

$$L^2(\mathbb{S}^{d-1}) = \bigoplus_{j=0}^{\infty} H_j^*(\mathbb{S}^{d-1}),$$

we can introduce spherical harmonic decomposition. Thus every $f \in L^2(\mathbb{S}^{d-1})$ has a unique representation of the form

$$f(\xi) = \sum_{j=0}^{\infty} \sum_{\ell=0}^{N_{j,d}} \hat{f}_{j,\ell} Y_{j,\ell}(\xi). \tag{4.5}$$

We call the coefficients $\hat{f}_{j,\ell}$ Fourier coefficients of f, they can be computed using the formula

$$\hat{f}_{j,\ell} = \langle f, Y_{j,\ell}\rangle_{\mathbb{S}^{d-1}}. \tag{4.6}$$

We also define the Sobolev space

$$W_2^\beta(\mathbb{S}^{d-1}) = \left\{ f \in L^2(\mathbb{S}^{d-1}) \middle| \ \|f\|^2_{W_2^\beta(\mathbb{S}^{d-1})} := \sum_{j=0}^{\infty} (1+\lambda_j)^\beta \sum_{\ell=0}^{N_{j,\ell}} |\hat{f}_{j,\ell}|^2 < \infty \right\},$$

where λ_j is the j-th eigenvalue of the Laplace-Beltrami operator on the sphere. The

Sobolev space is a Hilbert space with the scalar product

$$\langle f, g\rangle_{W_2^\beta(\mathbb{S}^{d-1})} = \sum_{j=0}^{\infty}\sum_{\ell=0}^{N_{j,d}}(1+\lambda_j)^\beta \hat{f}_{j,\ell}\hat{g}_{j,\ell}.$$

We are especially interested in the decomposition of spherical functions of the form $\varphi(\xi^T\zeta)$ with $\varphi : [-1,1] \to \mathbb{R}$ because our spherical basis functions are of this form. Their decomposition can be simplified using two basic results on spherical harmonics, the Addition theorem and the Funck-Hecke formula (quoted from [Mue66] Theorem 2, Theorem 5 and Theorem 6).

Theorem 4.2 (Addition Theorem)**.** *Let $\{Y_{j,\ell}\}$ be an orthonormal set of $N_{j,d}$ spherical harmonics of order j and dimension d. Then*

$$\sum_{\ell=1}^{N_{j,d}} Y_{j,\ell}(\xi)Y_{j,\ell}(\zeta) = \frac{N_{j,d}}{\omega_d}P_{j,d}(\xi^T\zeta),$$

where $P_{j,d}(t)$ is the Legendre polynomial of degree j and dimension d. This function can be given as Rodrigues' formula,

$$P_{j,d}(t) = \frac{(-1)^j\Gamma\left(\frac{d-1}{2}\right)}{2^j\Gamma\left(j+\frac{d-1}{2}\right)}(1-t^2)^{\frac{3-d}{2}}\frac{\partial^j}{\partial t^j}(1-t^2)^{j+\frac{(d-3)}{2}}, \quad -1 \le t \le 1.$$

Theorem 4.3 (Funck-Hecke formula)**.** *Suppose $\varphi(t)$ is continuous for $-1 \le t \le 1$. Then for every spherical harmonic of degree j*

$$\int_{\mathbb{S}^{d-1}} \varphi(\xi^T\zeta)Y_j(\zeta)\,d\omega_d(\zeta) = \hat{\varphi}(j)Y_j(\xi),$$

with

$$\hat{\varphi}(j) = \omega_{d-1}\int_{-1}^{1}\varphi(t)P_{j,d}(t)(1-t^2)^{\frac{d-3}{2}}\,dt. \tag{4.7}$$

Combining the last two theorems we can express every continuous $\varphi : [-1,1] \to \mathbb{R}$ in the form

$$\varphi(\xi^T\zeta) = \sum_{j=0}^{\infty}\sum_{\ell=0}^{N_{j,d}}\hat{\varphi}(j)Y_{j,\ell}(\zeta)Y_{j,\ell}(\xi) = \sum_{j=0}^{\infty}\frac{\hat{\varphi}(j)N_{j,d}}{w_d}P_{j,d}(\xi^T\zeta).$$

There are many different types of expansions used in the literature and each has advantages in some area of the theory. The coefficients $\hat{\varphi}(j)$ will be of importance for giving error estimates in Section 4.1.2. We will now introduce a second expansion which we will use in the next section to deduce the positive definiteness of basis functions. Since the described Legendre polynomials are seldom used, we will instead use the Gegenbauer polynomials, C_j^λ. Those are orthonormal polynomials with respect to the weight function $\omega(x) = (1-x^2)^{\lambda-\frac{1}{2}}$ on $[-1,1]$. Comparing their Rodrigues' formula to the above of the Legendre functions we find that

$$P_{j,d}(t) = \frac{k!\Gamma(d-2)}{\Gamma(k+d-2)} C_j^{\frac{d-2}{2}}(t) = \frac{1}{C_j^{\frac{d-2}{2}}(0)} C_j^{\frac{d-2}{2}}(t).$$

Resulting in an analogue of the Addition theorem and the Funck-Hecke Formula for Gegenbauer polynomials and an expansion of the form

$$\varphi(\xi^T\zeta) = \sum_{k=0}^{\infty} a_{k,d} C_k^\lambda(\xi^T\zeta), \quad \lambda = \frac{d-2}{2}, \tag{4.8}$$

with

$$a_{k,d} = \frac{1}{h_k^\lambda} \int_{-1}^{1} \varphi(x) C_k^\lambda(x)(1-x^2)^{\lambda-\frac{1}{2}}\, dx, \tag{4.9}$$

and

$$h_k^\lambda = \frac{C_k^\lambda(0)^2 \omega_d}{\omega_{d-1} N_{j,d}} = \int_{-1}^{1} (1-x^2)^{\lambda-\frac{1}{2}} \left(C_k^\lambda(x)\right)^2\, dx. \tag{4.10}$$

4.1.1 Interpolation on the sphere using radial basis functions

The spherical interpolation problem we now consider is similar to the one described in the first chapter of this thesis, except for the domain from which the data sites are stemming.

Problem 4.4. *Given a finite set $\Xi \subset \mathbb{S}^{d-1}$ of distinct points with corresponding function values $f(\xi) \in \mathbb{R}$, for $\xi \in \Xi$, stemming from a possibly unknown function $f : \mathbb{S}^{d-1} \to \mathbb{R}$, an interpolant $s : \mathbb{S}^{d-1} \to \mathbb{R}$ is to be computed satisfying*

$$s(\xi) = f(\xi), \quad \forall \xi \in \Xi.$$

As in the first chapter we want to form our interpolant as a linear combination of basis functions. These basis functions are now symmetric with respect to the geodesic distance to a given centre. Sometimes these functions are also referred to as zonal function. Such zonal function can easily be derived from a univariate function $\phi : [0,\pi] \to \mathbb{R}$ by inserting the geodesic distance to a certain centre. The interpolant is therefore of the form

$$s(x) = \sum_{\xi \in \Xi} c_\xi \phi(d(x,\xi)) + Y(x), \quad x \in \mathbb{S}^{d-1}, \quad Y \in H_k^+(\mathbb{S}^{d-1}), \tag{4.11}$$

$$\sum_{\xi \in \Xi} c_\xi \widetilde{Y}(\xi) = 0, \quad \text{for all } \widetilde{Y} \in H_k^+(\mathbb{S}^{d-1}).$$

This means we start using the enhanced interpolant because the interpolation without addition of spherical harmonics is included in this description when m is equal to zero.

As a criterion for the solvability of this problem we get an equivalent to conditionally positive definiteness in $\mathbb{R}^d$.

Definition 4.5. *A continuous function $\phi : [0,\pi] \to \mathbb{R}$ is* conditionally strictly positive definite of order m on the $d-$dimensional sphere *($CSPD_m(\mathbb{S}^{d-1})$), if and only if the matrix $A_\Xi = \{\phi(d(\xi,\zeta))\}_{\xi,\zeta \in \Xi}$ is positive definite on the space*

$$H_{m-1}^+(\mathbb{S}^{d-1}) \mid_\Xi^\perp := \left\{ \lambda \in \mathbb{R}^{|\Xi|} \middle| \sum_{\xi \in \Xi} \lambda_\xi Y(\xi) = 0, \ \forall \ Y \in H_{m-1}^+(\mathbb{S}^{d-1}) \right\}, \tag{4.12}$$

for all finite sets of distinct points $\Xi \subset \mathbb{S}^{d-1}$. If A_Ξ is only non-negative definite we call ϕ conditionally positive definite of order m *(CPD_m) on $\mathbb{S}^{d-1}$. If the former condition is satisfied for $m = 0$ we call the function* strictly positive definite on $\mathbb{S}^{d-1}$ *($SPD(\mathbb{S}^{d-1})$).*

We immediately see that

$$SPD(\mathbb{S}^{d-1}) \supset SPD(\mathbb{S}^{(d+1)-1}) \supset \cdots \supset SPD(\mathbb{S}^\infty)$$

and

$$SPD(\mathbb{S}^{d-1}) \subset CSPD_0(\mathbb{S}^{d-1}) \subset \cdots \subset CSPD_m(\mathbb{S}^{d-1}).$$

The interpolation has a unique solution of the described form for a $CSPD_m(\mathbb{S}^{d-1})$ function if the set of data sites Ξ includes an unisolvent subset (Definition 1.2) with respect to $H_k^+(\mathbb{S}^{d-1})$.

A first big step towards the characterisation of positive definite functions on the sphere is due to Schoenberg who in 1942 showed that every positive definite function has an expansion in Gegenbauer polynomials with non negative coefficients. To be precise we cite his result without proof from ([Sch42]).

Theorem 4.6 (Schoenberg)**.** *Every $\phi : [0, \pi] \to \mathbb{R}$ that is positive definite on $\mathbb{S}^{d-1}$ can be represented as*

$$\phi(\theta) = \sum_{k=0}^{\infty} a_{k,d} C_k^{\lambda}(\cos(\theta)), \qquad \theta \in [0, \pi], \tag{4.13}$$

where $a_{k,d} \geq 0$, for all k, $a_{k,d} \not\equiv 0$, and $\sum_{k=0}^{\infty} a_{k,d} < \infty$, $\lambda := (d-2)/2$, and finally the C_k^{λ} are the Gegenbauer polynomials.

The characterisation of the positive definite functions on spheres was completed by Chen, Menegatto and Sun [XC92]. They were able to state necessary and sufficient conditions for positive definite functions on spheres. Thereby we know that the positive definiteness of a function solely depends on the distribution of the coefficients $a_{k,d}$ with positive sign. We therefore define for a function $\phi \in CPD_m(\mathbb{S}^{d-1})$

$$K_{\phi} := \{k \in \mathbb{N}_m : a_{k,d} > 0\}, \tag{4.14}$$

and cite the following theorem from ([XC92], Theorem 3) without proof.

Theorem 4.7. *A function $\phi : [0, \pi] \to \mathbb{R}$ is strictly positive definite on the sphere $\mathbb{S}^{d-1}$ for $d \geq 3$ if and only if it is positive definite and K_{ϕ} includes infinitely many odd and infinitely many even integers.*

A characterisation of conditionally positive definite functions of higher order was given by Menegatto in [Men04]. We also cite his result without proof.

Theorem 4.8. *A continuous function $\phi : [0, \pi] \to \mathbb{R}$ is conditionally strictly positive definite of order m on $\mathbb{S}^{d-1}$ if and only if*

$$\phi(\theta) = \sum_{k=0}^{\infty} a_{k,d} C_k^{\lambda}(\cos(\theta)), \qquad \theta \in [0, \pi],$$

where $a_{k,d} \geq 0$ for all $k \geq m$, $\sum_{k=m}^{\infty} a_{k,d} < \infty$ and infinitely many coefficients $a_{k,d}$ with odd k and infinitely many coefficients with even k are positive.

We will from now on always refer to the function $\varphi : [-1, 1] \to \mathbb{R}$ as the function satisfying $\varphi(\xi^T \zeta) = \phi(d(\xi, \zeta))$. We will also say that such a function is in $CSPD_m(\mathbb{S}^{d-1})$ (or $CPD_m(\mathbb{S}^{d-1})$) if the corresponding ϕ is.

Many of the earlier results on spherical basis functions investigated the restrictions of Euclidean basis functions to the sphere. Some examples are [NSW07] and [HB01]. One important connection for the case of the surface spline was discovered by Hubbert and Morton in [HM04b], they noted a resemblance between the Fourier transform of the radial basis function ϕ in $\mathbb{R}^d$ and the Fourier coefficients of the spherical basis function on $\mathbb{S}^{d-1}$ (see Section 4.3). The connection was then established by Narcowich ([NSW07], Proposition 3.1.) we cite the result without proof.

Proposition 4.9. *Let $\Phi \in CSPD_m(\mathbb{R}^d)$ be a conditionally positive definite radial basis function having a generalised (d-dimensional) Fourier transform $\hat{\Phi}$ as in* (1.13) *that is measurable on $\mathbb{R}^d$. For the spherical basis function $\varphi(\xi^T\zeta) = \Phi(\xi - \zeta)|_{\xi,\zeta\in\mathbb{S}^{d-1}}$ and $j \geq 2m+1$ we have that*

$$\hat{\varphi}(j) = \int_0^\infty t\widehat{\Phi}(t)J_\nu^2(t)\,dt, \quad \nu := j + \frac{d-2}{2}, \tag{4.15}$$

where J_ν is the order ν Bessel function of the first kind.

4.1.2 The variational approach and some error estimates

We give a short introduction to the variational approach which was introduced by Madych and Nelson for the Euclidean setting. We state most of the theorems without proof and refer the reader to the paper [DNW99] of Dyn et al., where the approach is described in detail for the more general setting of interpolation on Riemannian manifolds. The results for Riemannian manifolds include as a special case the $(d-1)$-dimensional sphere for which the theorems are stated here. We also refer the reader to the recently published book by Hubbert et al. summing up the state of the art result on spherical radial basis functions [HLGM15].

The variational approach shows that the spherical basis function interpolant defined in the previous section is the norm minimizing interpolant in the so called native Hilbert space of the basis function.

The native space of a spherical basis function $\varphi \in CSPD_m(\mathbb{S}^{d-1})$ is defined as

$$H_{\varphi,m} := \left\{ f \in L^2(\mathbb{S}^{d-1}) \middle| \; \|f\|^2_{\varphi,m} := \sum_{j=m}^{\infty}\sum_{n=1}^{N_{j,d}} \frac{|\hat{f}_{j,n}|^2}{\hat{\varphi}(j)} < \infty \right\},$$

where $\hat{\varphi}(j)$ is as defined in (4.7). We note that $\|\cdot\|_{\varphi,m}$ is only a semi-norm with the spherical polynomials of order m as null space. Meaning that slight changes in the definition of the norm allow us to transform it into a native Hilbert space. By choosing any set $\{\xi_1, \ldots, \xi_n\} \subset \tilde{\Xi}$ that is unisolvent with respect to $H^+_{m-1}(\mathbb{S}^{d-1})$ we can define

$$H_\varphi := \left\{ f \in L^2(\mathbb{S}^{d-1}) \middle| \; \|f\|_\varphi^2 := \sum_{i=0}^{n} (f(\xi_i))^2 + \sum_{j=m}^{\infty} \sum_{n=1}^{N_{j,d}} \frac{|\hat{f}_{j,n}|^2}{\hat{\varphi}(j)} < \infty \right\},$$

which is a Hilbert space with the inner product

$$\langle f, g \rangle_\varphi = \sum_{i=1}^{n} f(\xi_i) g(\xi_i) + \sum_{j=m}^{\infty} \sum_{n=1}^{N_{j,d}} \frac{\hat{f}_{j,n} \hat{g}_{j,n}}{\hat{\varphi}(j)}.$$

The following optimal recovery result is true in a much more general setting including the Euclidean space. It is described in detail in [Sch99].

Theorem 4.10 (Optimal interpolation in the native space)**.** *Let $\Xi \subset \mathbb{S}^{d-1}$ be a finite set of distinct points containing a unisolvent subset Ξ with respect to $H^+_{m-1}(\mathbb{S}^{d-1})$ and $\varphi \in CSPD_m(\mathbb{S}^{d-1})$. Then the solution of the φ-based interpolation of the form* (4.11) *solves*

$$\text{minimise}\{\|s\|_\varphi \;:\; s \in H_\varphi \text{ and } s(\xi) = f(\xi),\ \forall \xi \in \Xi\}.$$

For a given $f \in H_\varphi$ let s_f denote the optimal φ-based spherical basis function interpolant to f, then

1. $\|f - s_f\|_\varphi^2 = \langle f, f - s_f \rangle_\varphi$,
2. $\|f - s_f\|_\varphi \leq \|f\|_\varphi$.

Since it is of special interest that the error estimates and optimal approximation property not only apply to the native spaces but to the Sobolev spaces defined in the previous section we mention here an important property of norm equivalence. The structure of the native space depends on the decay of the Fourier coefficients of the basis function, so a property is introduced to describe the decay of those coefficients.

Definition 4.11. *We say φ has α-Fourier decay, when there are positive constants A_1, A_2, s.t.*

$$A_1(1+j)^{-(d-1+\alpha)} \leq \hat{\varphi}(j) \leq A_2(1+j)^{-(d-1+\alpha)}, \quad \alpha > 0, \quad j \geq m. \tag{4.16}$$

This only applies to functions whose coefficients decay at a polynomial rate; for those functions we can deduce a connection to Sobolev spaces. The Sobolev space $W_2^\beta(\mathbb{S}^{d-1})$ described in the previous section is the native space of the kernel with Fourier coefficient

$(1+\lambda_k)^{-\beta} = \left(1+j^2+(d-2)j\right)^{-\beta}$ which are of $\alpha = 2\beta - d + 1$-Fourier decay. One can immediately see that the native Hilbert space of $\varphi \in CSPD_0(\mathbb{S}^{d-1})$ with α-Fourier decay is norm equivalent to the Sobolev space W_2^β with $\beta = (d-1+\alpha)/2$.

Example 4.12.

- *We will in Section 4.3 give the Fourier coefficients of the surface spline introduced by Hubbert in [HM04b]. The basis function is for $d = 3$*

$$\varphi(x) = (-1)^m (2-2x)^{\left(\frac{m-2}{2}\right)} \log(2-2x), \quad x \in [-1,1], \tag{4.17}$$

and its native space is the Sobolev space $W_2^{2m}(\mathbb{S}^2)$.

- *In [NW02] Narcowich et al. show that the restriction of the compactly supported Wendland basis functions to the sphere have native spaces which are Sobolev spaces. One example is*

$$\psi_{3,1}(r) = (1-r)_+^4(4r+1), \quad r \in \mathbb{R}_{\geq 0}$$

which satisfies $\psi \in C^2(\mathbb{R}^3)$ and its restriction to the sphere

$$\varphi(\xi^T\nu) = \psi_{3,1}\left(\sqrt{2-2\xi^T\nu}\right)|_{\xi,\nu\in\mathbb{S}^2}$$

satisfies $H_\varphi = W_2^{2.5}(\mathbb{S}^2)$.

For functions whose coefficients decay at an exponential rate the optimal recovery of Theorem 4.10 only applies to a significantly smaller space of functions.

4.1.3 Local and global error estimates

To develop error estimates, the mesh distance between two points is an important tool. It is also sometimes referred to as the separation distance and we will denote it by

$$h_\Xi := \sup_{\zeta\in\mathbb{S}^{d-1}} \min\{d(\zeta,\xi) : \xi \in \Xi\}.$$

One of the first error estimates for spherical interpolation was given by Jetter, Stöckler and Ward in [JSW99]. More recent estimates are relying on the same idea: Let $\Xi \subset \mathbb{S}^{d-1}$ contain a unisolvent subset with respect to $H_{m-1}^+(\mathbb{S}^{d-1})$. To compute this error estimate at one fixed site $\zeta \in \mathbb{S}^{d-1}$, we choose coefficients γ_ξ, $\xi \in \Xi$, such that

$$Y(\zeta) = \sum_{\xi\in\Xi} \gamma_\xi Y(\xi), \quad \forall\, Y \in H_{m-1}^+(\mathbb{S}^{d-1}). \tag{4.18}$$

We can now define the bounded linear functional

$$\Lambda_\zeta(f) = \left(\delta_\zeta - \sum_{\xi\in\Xi}\gamma_\xi\delta_\xi\right)(f), \quad \forall f \in H_\varphi.$$

Since the interpolation error satisfies $(f - s_f)(\xi) = 0$ for all $\xi \in \Xi$, we can use this functional to deduce

$$|f(\zeta) - s_f(\zeta)| = |\Lambda_\zeta(f - s_f)| = |\langle k_{\Lambda_\zeta}, f - s_f\rangle| \leq \|k_{\Lambda_\zeta}\|_\varphi \|f - s_f\|_\varphi, \tag{4.19}$$

where k_{Λ_ζ} is the Riesz representation of Λ_ζ and the last inequality follows using the Cauchy-Schwarz inequality. The factor $\|k_{\Lambda_\zeta}\|_\varphi$ is called a powerfunction for φ at ζ and is denoted as $P_{\varphi,\gamma}(\zeta) = \|k_{\Lambda_\zeta}\|_\varphi$. An expression for the powerfunction was computed in 1999 by Levesley et al. [LLRS99]. They use the Riesz representation theorem from which

$$\|k_{\Lambda_\zeta}\|_\varphi^2 = \Lambda_\zeta(k_{\Lambda_\zeta}) = P_{\varphi,\gamma}(\zeta)^2$$

follows. From this the representation

$$P_{\varphi,\gamma}(\zeta) = \left(\sum_{\xi\in\Xi}\sum_{\eta\in\Xi}\gamma_\xi\gamma_\eta\varphi(\xi^T\eta) - 2\sum_{\xi\in\Xi}\gamma_\xi\varphi(\xi^t\zeta) + \varphi(1)\right)^{\frac{1}{2}},$$

can be deduced. The value of the powerfunction at ζ depends on the chosen parameters γ_ξ, so it is a goal to find the powerfunction with smallest norm $\|k_{\Lambda_\zeta}\|_\varphi$. By enlarging the set Ξ so that $\Xi_0 = \Xi \cup \{\zeta\}$ and setting $\gamma_\zeta = -1$ we can rewrite the powerfunction:

$$P_{\varphi,\gamma}(\zeta) = \left(\sum_{\xi\in\Xi_0}\sum_{\eta\in\Xi_0}\gamma_\xi\gamma_\eta\varphi(\xi^T\eta)\right)^{\frac{1}{2}} = \left\|\sum_{\xi\in\Xi_0}\gamma_\xi\delta_\xi\right\|_{\varphi*}.$$

Definition 4.13. *We define the optimal powerfunction for φ at ζ as*

$$P_{\varphi,\gamma*}(\zeta) = \min\left\{\left\|\sum_{\xi\in\Xi_0}\gamma_\xi\delta_\xi\right\|_{\varphi*} : \{\gamma_\xi\}_{\xi\in\Xi} \text{ satisfy } (4.18) \text{ and } \gamma_\zeta = -1\right\},$$

where $\|\cdot\|_{\varphi*}$ is the dual space norm given by $\|T\|_{\varphi*} = \sup\{|Tf| : \|f\|_\varphi \leq 1\}$.

Computing the optimal powerfunction is not necessary to derive error estimates. We therefore are content to find an upper bound on the norm of the powerfunction so we can estimate the error of the interpolation in ζ using (4.19). To do so we use a property described by Jetter et al. in [JSW99].

Lemma 4.14. *Let $\Xi \subset \mathbb{S}^{d-1}$ be any finite and distinct point set with mesh norm h_Ξ, and let K be the positive integer K satisfying*

$$\frac{1}{K+1} \leq 2h_\Xi \leq \frac{1}{K}. \tag{4.20}$$

Then there exists $\gamma \in \mathbb{R}^\Xi$, $\|\gamma\|_1 \leq 2$, so that for any $\zeta \in \mathbb{S}^{d-1}$ (4.18) holds for $K = m-1$.

We can use this coefficient vector γ to define one powerfunctions for φ, whose norm we can easily estimate. The following theorem is taken from [HLGM15], but the error estimate is easily computable using the inequality (4.19) and the Fourier decay of φ together with the coefficients γ of the previous lemma.

Theorem 4.15. *Let $\Xi \subset \mathbb{S}^{d-1}$ be a finite set with mesh norm h_Ξ, satisfying (4.20) for some $K \geq m-1$, $\varphi \in CSPD_m(\mathbb{S}^{d-1})$ with an α-Fourier decay property. Then for any $f \in H_\varphi$ the spherical basis function interpolant s_f satisfies for any $\zeta \in \mathbb{S}^{d-1}$*

$$|f(\zeta) - s_f(\zeta)| \leq C \cdot h_\Xi^{\alpha/2} \|f - s_f\|_\varphi,$$

where C is a positive constant independent of h_Ξ.

Applying Duchon's technique to the sphere, Hubbert et al. were able to construct global error bounds from these local error estimates. The technique basically consists of three steps (those are the same in Euclidean and spherical contexts):

1. Construct a scalable mesh for the domain, so that you get a collection of sites $\Omega \subset \mathbb{S}^{d-1}$ for which the open balls $B_i = B(x_i, h)$, $x_i \in \Omega$, cover the domain and have uniformly bounded overlap.

2. Estimate the local approximation error in the areas B_i.

3. Extend the results for the balls to the whole domain and then estimate the error on the whole domain by gluing the results together.

For the details of the proof which involves some geometric construction of the mesh, and construction of extension operators for the local Sobolev spaces we refer the reader to [HLGM15]. From this book we cite the following theorem without proof (Theorem 3.4).

Theorem 4.16. *Let $\varphi \in CSPD_m(\mathbb{S}^{d-1})$ be a spherical basis function having α-Fourier decay for $\alpha > 0$, $f \in H_\varphi$ and s_f be the φ-based interpolant to f on the set $\Xi \subset \mathbb{S}^{d-1}$ with separation distance h_Ξ. There exists a positive number h_0 such that, if $h_\Xi \in (0, h_0)$ then the following holds*

$$\|s_f - f\|_{L^p(\mathbb{S}^{d-1})} = \begin{cases} \mathcal{O}\left(h_\Xi^{\frac{\alpha}{2}+\frac{d-1}{p}}\right), \ p \in [2, \infty]; \\ \mathcal{O}\left(h_\Xi^{\frac{\alpha}{2}+\frac{d-1}{2}}\right), \ p \in [1, 2). \end{cases} \tag{4.21}$$

4.2 Monotone functions and spherical interpolation

In this section we demonstrate how monotonicity properties can be used to prove positive definiteness on the sphere. In the first chapter of this thesis we stated the known results for the Euclidean basis functions; to be able to do the same for the sphere we will need to show that the Gegenbauer coefficients of a basis function are positive. The Gegenbauer coefficients (defined in (4.9)) of a function $\phi : [0, \pi] \to \mathbb{R}$, satisfying $\varphi(\xi^T \zeta) = \phi(d(\xi, \zeta))$, for $\lambda > 0$, are given by

$$\begin{aligned} a_{k,d} &= \frac{1}{h_k^\lambda} \int_{-1}^{1} \varphi(x) C_k^\lambda(x)(1-x^2)^{\lambda-\frac{1}{2}}\, dx \\ &= \frac{1}{h_k^\lambda} \int_{0}^{\pi} \phi(\theta) C_k^\lambda(\cos(\theta))(\sin(\theta))^{2\lambda}\, d\theta, \end{aligned}$$

where

$$h_k^\lambda = \int_{-1}^{1} \left(C_k^\lambda(t)\right)^2 (1-t^2)^{\lambda-\frac{1}{2}}\, dt \geq 0. \tag{4.22}$$

For functions which are positive definite on spheres of arbitrary dimension (and thereby on $\mathbb{S}^\infty$) Schoenberg derived a simple representation in [Sch42]. The characterisation of strictly positive definite functions on $\mathbb{S}^\infty$ was later completed by Menegatto in [Men94], we cite his result without proof.

Theorem 4.17. *A function ϕ is strictly positive definite on $\mathbb{S}^{d-1}$ for all $d > 1$ if and only if it has the form*

$$\phi(\theta) = \sum_{m=0}^{\infty} a_m (\cos(\theta))^m, \tag{4.23}$$

where $a_m \geq 0$ for all m, $0 \neq \sum_{m=0}^{\infty} a_m < \infty$ and $a_m > 0$ for infinitely many even and infinitely many odd values of m. The positive definite functions on the Hilbert sphere $\mathbb{S}^\infty$ can also be represented as an infinite series in this form.

From this representation we can immediately deduce that, a positive definite function $\varphi : [-1, 1] \to \mathbb{R}$ on $\mathbb{S}^\infty$ must have the form

$$\varphi(x) = \phi(\arccos(x)) = \sum_{m=0}^{\infty} a_m\, x^m,$$

and be absolutely monotone on $[0, 1]$.

Furthermore, if a function $\widetilde{\phi}$ is conditionally positive definite of order m on $\mathbb{R}^d$ for all dimensions d, then we have that

$$g(\cdot) = \widetilde{\phi}(\sqrt{\cdot})$$

is completely monotone of order m (see Theorem 1.14). Using the connection of the Euclidean distance and the geodesic distance, $\|\xi - \zeta\| = \sqrt{2 - 2\xi^T\zeta}$, we get that the restriction of this basis function $\widetilde{\phi}$ to the sphere, dependent on the inner product is

$$\varphi(\cdot) = \widetilde{\phi}\big(\sqrt{2 - 2\cdot}\big) = g(2 - 2\cdot).$$

The function φ is obviously conditionally positive definite of order m on $\mathbb{S}^{d-1}$ under the assumptions above. It follows using the arguments as described in Section 3 that if g is completely monotone of order m on $[0, \infty)$, then φ will be completely absolutely monotone of order m on $(-\infty, 1]$ (meaning $\psi^{(m)}$ is absolutely monotone). This gives us an additional reason to investigate the monotonicity of φ. The latter argument can be reversed and gives a criterion for positive definiteness on all spheres. The theorem was also proven by zu Castell (as is known from private communication, 2017).

Theorem 4.18. *For all $\varphi \in C((-\infty, 1])$ that are absolutely monotone of order m on $(-\infty, 1)$ (meaning $\varphi^{(m)}$ is absolutely monotone on $(-\infty, 1)$), $\varphi(\cos(\cdot))$ is strictly conditionally positive definite of order m on $\mathbb{S}^{d-1}$ for all d.*

For $m = 0$ the function is even strictly positive definite and according to Theorem 1.12 the functions with $m = 1$ will result in non singular interpolation matrices if $\widetilde{\phi}(0) \leq 0$.

We note that the absolute monotonicity implies that φ is analytic in $(-1, 1)$, because it possesses the series expansion described in Theorem 4.17. The connection between the monotonicity of a function and this function being analytic was first described by Bernstein and later proven in a more general setting by McHugh [McH75], we cite a further generalisation of Cater ([Cat99], Theorem I) without proof.

Definition 4.19. *We say a function $f : (a, b) \to \mathbb{R}$ is* regularly monotonic *if $f \in C^\infty((a, b))$ and each derivative is of a fixed sign.*

This definition includes completely monotonicity as well as absolute monotonicity.

Theorem 4.20. *If f is regularly monotonic on $(-a, a)$, then for any $x \in (-a, a)$ we have*

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} x^n.$$

Before we apply this theorem we first note: the analogue of Theorem 4.18 for n-times absolutely monotone functions is not true, as is to be seen in the next (counter-)example.

Example 4.21. *The function $\varphi(x) = x_+^{\mu-1}$ is n-times absolute monotone on $(-\infty, 1]$ for μ larger than n, but $\varphi(\cos(x))$ is not positive definite. The $(\mu+2)$-nd coefficients in the Gegenbauer expansion can be computed as*

$$\begin{aligned} a_{\mu+2,d} &= \frac{1}{h_{\mu+2}^{\lambda}} \int_{-1}^{1} \varphi(x) C_{\mu+2}^{\lambda}(x)(1-x^2)^{\lambda-\frac{1}{2}}\, dx \\ &= \frac{(\mu+2+\lambda)(\mu+2)!\Gamma(\lambda)2^{-\mu}\Gamma(\mu)}{\Gamma(\frac{3}{2}+\mu+\lambda)\Gamma(-\frac{1}{2})} \\ &= -\frac{(\mu+2+\lambda)(\mu+2)!\Gamma(\lambda)\Gamma(\mu)}{\Gamma(\frac{3}{2}+\mu+\lambda)2^{\mu+1}\sqrt{\pi}} < 0, \end{aligned}$$

according to (18.17.37) in [OOL$^+$18] together with (4.10)*. The negativity mentioned in the last display is due to the negative factor of the gamma function* $\Gamma(-1/2) = -2\sqrt{\pi}$ *in the denominator.*

Now, however, we shall see that it is also possible to get a monotonicity result for finite (multiple) monotonicity.

Lemma 4.22. *If*

$$\widetilde{\phi}(x) = \varphi\left(1 - \frac{x^2}{2}\right), \qquad x \geq 0, \tag{4.24}$$

is n-times monotone on $(0, \infty)$ *and no polynomial, then* $\varphi\Big(\cos(\cdot)\Big)$ *is strictly positive definite on $\mathbb{S}^{d-1}$ so long as $n \geq \lfloor d/2 \rfloor + 2$.*

Proof. According to Theorem 1.24, $\widetilde{\phi}$ is strictly positive definite on $\mathbb{R}^d$ for $n \geq \lfloor d/2 \rfloor + 2$ and so is its restriction to the sphere which can also be represented as

$$\tilde{\phi}\left(\sqrt{2 - 2\cos(\theta)}\right) = \varphi\Big(\cos(\theta)\Big).$$

This is strictly positive definite on $\mathbb{S}^{d-1}$ for $d \leq 2n-3$. Thus, according to the definition of the lower brackets, the integral part of $d/2$ must be at most $n-2$. □

Using the computation of the coefficients of the expansion we can show another sufficient condition for positive definiteness on all spheres.

Theorem 4.23. *Let $\varphi \in C^\infty([-1,1])$ be absolutely monotone of order m on $[-1,1]$ and let it be no polynomial. Then the function $\varphi(\cos(\cdot))$ is conditionally strictly positive definite of order m on $\mathbb{S}^{d-1}$ for all $d \geq 3$.*

Proof. We compute the coefficients $a_{k,d}$ of the function $\varphi\big(\cos(\cdot)\big)$ repeatedly (by k-fold) applying integration by parts, namely, using the Pochhammer symbol $(\cdot)_k$,

$$\begin{aligned}
a_{k,d} &= \frac{1}{h_k^\lambda}\int_{-1}^{1}\varphi(x)C_k^\lambda(x)(1-x^2)^{\lambda-\frac{1}{2}}\,dx \\
&= \frac{1}{h_k^\lambda}\int_{-1}^{1}\varphi(x)\frac{(2\lambda)_k}{(-2)^k(\lambda+\frac{1}{2})_k k!}\frac{\partial^k}{\partial x^k}(1-x^2)^{k+\lambda-\frac{1}{2}}\,dx \\
&= \frac{1}{h_k^\lambda}\int_{-1}^{1}\frac{(2\lambda)_k}{2^k(\lambda+\frac{1}{2})_k k!}\varphi^{(k)}(x)(1-x^2)^{k+\lambda-\frac{1}{2}}\,dx > 0, \quad \text{for all } k \geq m.
\end{aligned}$$

This establishes the assertion according to Schoenberg's famous results quoted as Theorem 4.6 and Theorem 4.8. □

This gives another sufficient condition for (conditionally) positive definiteness on all spheres which is easy to evaluate. Allowing us to give a number of new conditionally positive definite basis functions, for example the function class $\psi(x) = (-1)^m(2-x)^{m-\epsilon}$, where $m \in \mathbb{N}$ and $\epsilon \in [0,1)$, which is absolutely monotone of order m and therefore conditionally positive definite of order m on $\mathbb{S}^{d-1}$ for any $d \geq 3$.

From Theorem 4.17 it follows that all functions which are strictly positive definite on $\mathbb{S}^\infty$ are absolutely monotone on the interval $[0,1]$ and are no polynomials, the monotonicity is in this case necessary but not sufficient. One counter-example would be the function

$$\sum_{k=0}^{\infty}\frac{1}{k!}x^{2k} \tag{4.25}$$

which is absolutely monotone but does not satisfy the condition of Menegatto, cited as Theorem 4.17, for strictly positive definite functions on the Hilbert sphere.

A sufficient condition for conditionally strictly positive definiteness of order m on spheres of arbitrary dimension, derived from Theorem 4.8, is as follows.

Lemma 4.24. *Any function $\psi : [-1,1] \to \mathbb{R}$ which has a representation for all arguments of the form*

$$\psi(x) = \sum_{k=0}^{\infty} a_k x^k,$$

where $a_k \geq 0$ for $k \geq m$ and $a_k > 0$ for infinitely many even and infinitely many odd values of k, is conditionally strictly positive definite of order m on $\mathbb{S}^{d-1}$ for all $d > 2$.

Proof. The result follows immediately from Lemma 1 of the paper [Bin73], where the relation

$$x^n = \frac{n!\Gamma(\lambda)}{2^n\Gamma(2\lambda)} \sum_{0\le 2k\le n} \frac{(n-2k+\lambda)\Gamma(n-2k+2\lambda)}{k!(n-2k)!\Gamma(n-k+\lambda+1)} \frac{C^{\lambda}_{n-2k}(x)}{C^{\lambda}_{n-2k}(1)}$$

is established for all positive λ, and the factors of the Gegenbauer coefficients are all positive for $\lambda \ge 0$.

□

We now turn to the investigation of the monotonicity properties of the functions

$$\phi : [0,\pi] \to \mathbb{R}$$

dependent on the geodesic distance. Most recently Gneiting, Beatson et al., stated Pólya criteria for positive definiteness of functions on the sphere. Here is a short list of available results.

- Beatson et al., in [BzCX14] stated in a conjecture a sufficient condition for all d for the positive definiteness of compactly supported basis functions, which they proved for $d \le 8$.

- Gneiting in [Gne13] generalised the conjecture for functions that are not compactly supported, and he proved it furthermore for $d \le 8$.

- Both conjectures can now be proven using the results of Xu [Xu18]. The article includes the proof of Beatson et al.'s conjecture.

We state the result for multiply monotone functions which is a slight change to the conjecture of Gneiting (Theorem 6 in [Gne13] for $d \le 3$), and we shall give the proof using the result of Xu.

Theorem 4.25. *Suppose that $\phi \in C^{n-2}([0,\infty))$ is n-times monotone and not constant. Then its restriction $\phi|_{[0,\pi]}$ is strictly positive definite on $\mathbb{S}^{2n-1}$.*

Proof. Using the Williamson representation in the computation of the Gegenbauer coefficients we get

$$
\begin{aligned}
a_{k,d} &= \frac{1}{h_k^\lambda}\int_0^\pi \phi(\theta) C_k^\lambda(\cos(\theta))(\sin(\theta))^{2\lambda}\, d\theta \\
&= \frac{1}{h_k^\lambda}\int_0^\pi \int_0^{\frac{1}{\theta}} (1-\theta\beta)_+^{n-1} d\gamma(\beta) C_k^\lambda(\cos(\theta))(\sin(\theta))^{2\lambda}\, d\theta \\
&= \frac{1}{h_k^\lambda}\int_0^\infty \int_0^{\pi} (1-\theta\beta)_+^{n-1} C_k^\lambda(\cos(\theta))(\sin(\theta))^{2\lambda}\, d\theta\, d\gamma(\beta) \\
&= \frac{1}{h_k^\lambda}\int_{\frac{1}{\pi}}^\infty \underbrace{\int_0^{\frac{1}{\beta}} (1-\theta\beta)^{n-1} C_k^\lambda(\cos(\theta))(\sin(\theta))^{2\lambda}\, d\theta\, d\gamma(\beta)}_{(\star\star)} \\
&+ \frac{1}{h_k^\lambda}\int_0^{\frac{1}{\pi}} \underbrace{\int_0^{\pi} (1-\theta\beta)^{n-1} C_k^\lambda(\cos(\theta))(\sin(\theta))^{2\lambda}\, d\theta\, d\gamma(\beta)}_{(\star\star\star)},
\end{aligned}
$$

where we have also used the definition of the truncated power functions.

Expression $(\star\star)$ was shown to be strictly positive for $n-1 \geq \lambda+1$ in [Xu18], Theorem 2, and the function we are talking about is therefore positive definite on $\mathbb{S}^{2n-1}$. Moreover, the part $(\star\star\star)$ is positive because the functions $\phi(t) = (1-\theta t)_+^n$ are positive definite on the sphere $\mathbb{S}^{d-1}$ for all d if $\theta < \frac{1}{\pi}$ [Gne13]. $\square$

We also cite a result of Gneiting concerning completely monotonic functions ([Gne13], Theorem 7).

Theorem 4.26. *Suppose that the function $\phi : [0,\infty) \to \mathbb{R}$ is completely monotone on $(0,\infty)$ with $\phi(0) = 1$ and not constant. Then the restriction $\widetilde{\phi} = \phi|_{[0,\pi]}$ is positive definite on the sphere $\mathbb{S}^{d-1}$ for any $d \geq 2$.*

We give a alternative condition which requires only the completely monotonicity on the interval $[0, \frac{\pi}{2}]$ while imposing slightly stronger conditions on the smoothness of the function.

Theorem 4.27. *Let $\phi : [0,\pi] \to \mathbb{R}$ be a function which can be represented as a convergent power series with centre at $\frac{\pi}{2}$, if ϕ is completely monotonic on $[0,\pi/2]$ and $\phi^{(j)}(\frac{\pi}{2}) \neq 0$ for at least one $j > 1$ even and at least one $j > 0$ odd, then ϕ is strictly positive definite on $\mathbb{S}^{d-1}$ for any $d \geq 3$.*

Proof. We can represent the function as

$$
\phi(\theta) = \sum_{j=0}^\infty \frac{1}{j!}\phi^{(j)}\left(\frac{\pi}{2}\right)\left(\theta - \frac{\pi}{2}\right)^j, \quad \text{with } (-1)^j \phi^{(j)}\left(\frac{\pi}{2}\right) \geq 0,
$$

because of the required monotonicity. Then we compute the series representation of $\psi(x) = \phi(\arccos(x))$, $x \in [-1,1]$, using the power series of the

$$\arccos(x) = \frac{\pi}{2} - \sum_{k=0}^{\infty} \frac{1}{k!}\binom{2k}{k}\frac{x^{2k+1}}{4^k(2k-1)}.$$

It follows that

$$\psi(x) = \phi(\arccos(x)) = \sum_{j=0}^{\infty} \frac{1}{j!}\phi^{(j)}\left(\frac{\pi}{2}\right)\left(-\sum_{k=0}^{\infty}\frac{1}{k!}\binom{2k}{k}\frac{x^{2k+1}}{4^k(2k-1)}\right)^j = \sum_{\ell=0}^{\infty} a_\ell x^\ell.$$

And now it follows that $a_\ell > 0$ from

$$(-1)^j\phi^{(j)}\left(\frac{\pi}{2}\right) > 0$$

for at least one even and one odd value of j. The summability of the coefficients follows from the convergence radii of the functions. □

Theorem 4.28. *If $\phi \in C([0,\pi])$ is completely monotone on $(0,\pi)$, then it is sufficient for the strict positive definiteness on $\mathbb{S}^\infty$ that $\phi \notin \mathbb{P}^1|_{[0,\pi]}$.*

Proof. Since ϕ is completely monotone on $(0,\pi)$, $\phi\left(\cdot + \frac{\pi}{2}\right)$ will be completely monotone on $(-\frac{\pi}{2}, \frac{\pi}{2})$. Applying Theorem 4.20 we find a representation

$$\phi\left(\theta + \frac{\pi}{2}\right) = \sum_{n=0}^{\infty}\frac{\phi(\frac{\pi}{2})}{n!}\theta^n, \quad \theta \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right),$$

which implies that it possesses the representation necessary to apply Theorem 4.27. □

This theorem also allows us to give an alternative proof for the positive definiteness of the function class $\phi(\theta) = (1-\theta\beta)_+^n$ for $\beta < \frac{1}{\pi}$, $n \geq 2$. The original proof of Gneiting ([Gne13]) made use of a convolution argument.

We can now also give a result for completely monotone functions of order one.

Theorem 4.29. *1. Let $\phi : [0,\pi] \to \mathbb{R}$ be a function which can be represented as a convergent power series with centre at $\pi/2$. If ϕ is completely monotonic of order 1 on $[0,\pi/2]$ and $\phi^{(j)}(\frac{\pi}{2}) \neq 0$ for at least one even and one odd value of $j \in \mathbb{N}$, then ϕ is conditionally strictly positive definite of order one on $\mathbb{S}^{d-1}$ for any $d \geq 3$.*

2. If, on top of the conditions of (1), the function is non-positive at the origin, the according interpolation matrix will be non-singular even without any constants added *to the interpolant and without side-conditions.*

Proof. For a function ϕ as described we can define the function $\widetilde{\phi}(\theta) = \phi(\theta) - \phi\left(\frac{\pi}{2}\right)$, then Theorem 4.27 applies to $\widetilde{\phi}$ which therefore is strictly positive definite for arbitrary dimensions d. Also

$$\widetilde{\psi}(x) = \widetilde{\phi}(\arccos(x)) = \sum_{\ell=1}^{\infty} a_\ell x^\ell = \psi(x) - \phi\left(\frac{\pi}{2}\right),$$

and thereby $\psi(x) = \sum_{\ell=1}^{\infty} a_\ell x^\ell + \phi\left(\frac{\pi}{2}\right)$ and ϕ is conditionally positive definite of order one according to Lemma 4.24.

For the statement (2) about $\phi(0) \leq 0$, that the according interpolation matrix will be non-singular even without any constants added to the interpolant and without side-conditions, see the classical argument: the trace of the interpolation matrix is non-positive, therefore so is the sum of its eigenvalues, and thus – all but one eigenvalue being positive – the missing one must be negative. Thus the interpolation matrix is regular. □

We can again avoid the condition on the power series expansion which is harder to test by making use of Theorem 4.20.

Theorem 4.30. *Let $\phi : [0, \pi] \to \mathbb{R}$ be a function which is completely monotone of order 1 on $[0, \pi]$, $\phi''(\frac{\pi}{2}) \neq 0$ and $\phi(t) \neq 0$, $\forall t \in [0, \pi]$ then ϕ is conditionally strictly positive definite of order one on $\mathbb{S}^{d-1}$ for any $d \geq 3$.*

Proof. From Theorem 4.20 we can deduce that the function has a series expansion of the form required in Theorem 4.29. The conditionally positive definiteness of order one follows from this theorem. □

Example 4.31. *One radial basis function that has the aforementioned regularity properties for interpolation derived from this theorem is the function*

$$\phi(\theta) = -\sqrt{\frac{1}{\pi}}\left(\frac{\pi}{2} + \theta\right)^{1/2} = -\sqrt{\frac{1}{\pi}}\left(\left(\theta - \frac{\pi}{2}\right) + \pi\right)^{1/2} = -\left(\frac{\theta - \pi/2}{\pi} + 1\right)^{1/2} \tag{4.26}$$

which has the power series representation

$$\phi(\theta) = -\sum_{j=0}^{\infty} \binom{0.5}{j} \left(\frac{1}{\pi}\right)^j \left(\theta - \frac{\pi}{2}\right)^j,$$

the binomial coefficient $\binom{0.5}{j}$ being of course $\frac{\Gamma(3/2)}{j!\Gamma(3/2-j)}$.

Example 4.32. *We can now characterise the class of polynomials* $p \in \mathbb{P}^2|_{[0,\pi]}$ *which satisfy* $p \in SPD(\mathbb{S}^\infty)$*. Namely,*

$$p(\theta) = a\theta^2 + b\theta + c \in SPD(\mathbb{S}^d)$$

if and only if

$$a > 0, \quad b < -\pi a, \quad c \geq -\frac{\pi}{2}\left(\frac{\pi}{2}a + b\right).$$

We can also show some conditions on ϕ which are necessary, for all ϕ which are positive definite for arbitrary d.

Lemma 4.33. *For* $\phi : [0,\pi] \to \mathbb{R}$ *to be strictly positive definite on all spheres it is necessary that* $\phi \in C^\infty((0,\pi))$ *and* ϕ *once monotone on* $(0,\pi/2]$*.*

Proof. Since for every positive definite ϕ, ϕ has an absolutely convergent power series expansion in the variable $\cos(\cdot)$ we deduce that $\phi \in C^\infty((0,\pi))$. Also we saw in Theorem 4.17 that it is necessary that φ is absolutely monotone on $[0,1)$. Since

$$\varphi(x) = \phi(\arccos(x)) \geq 0$$

for $x \in [0,1)$ we need that $\phi(\theta) \geq 0$ for $\theta \in (0,\pi/2]$ because the image of $[0,1)$ under the arccos is $(0,\pi/2]$. Also

$$\varphi'(x) = \phi'(\arccos(x)) \cdot \arccos'(x) \geq 0, \quad \forall x \in [0,1)$$

can only be satisfied if $\phi'(\theta) \leq 0$ for $\theta \in (0,\pi/2]$ since $\arccos'(x) \leq 0$ for $x \in [0,1)$. $\square$

4.2.1 Summary of the results

We want to be better able to compare the results of the last section and also discuss whether the given monotonicity properties are sufficient or necessary or possible both. We will in this section visualize the results of the last section and add examples for 'non sufficients' or 'non necessity' where missing. As is obvious the majority of the achieved results are only sufficient, but as Askey stated [Ask75].

> "It is an unfortunate fact that necessary and sufficient conditions are often impossible to verify and one must search for useful sufficient conditions when confronted with a particular example."

Function	Monotonicity conditions	Necessary	Sufficient	Proofs/Examples
$\varphi : [-1,1] \to \mathbb{R}$	Absolutely monotone on $[0,1)$	YES	NO	Theorem 4.17 / Equation (4.25)
$\varphi \in C^\infty([-1,1])$ no polynomial	Absolutely monotone on $[-1,1]$	NO	YES	Theorem 4.23/Example 4.34
$\phi : [0,\pi] \to \mathbb{R}$, $\phi \in C^\infty((0,\pi))$, $\phi \not\equiv$const	once monotone on $(0,\pi/2]$	YES	NO	Lemma 4.33/ Example 4.35
$\phi : [0,\infty) \to \mathbb{R}$, $\phi(0)=1$, $\phi \not\equiv$const	Completely monotone on $(0,\infty)$	NO	YES	Theorem 4.26 / Example 4.36
$\phi : [0,\pi] \to \mathbb{R}$, $\phi \notin \mathbb{P}^1$	Completely monotone on $[0,\pi]$	NO	YES	Theorem 4.28/ Example 4.36
$\phi : [0,\pi] \to \mathbb{R}$, see for additional conditions Theorem 4.27	Completely monotone on $[0,\pi/2]$		YES	Theorem 4.27

Table 4.1: Table of monotonicity conditions for strictly positive definite functions on arbitrary spheres

Function	Monotonicity conditions	Necessary	Sufficient	Proofs/Examples
$\varphi \in C^\infty([-1,1])$, no polynomial	Absolute monotone of order m on $[-1,1]$	NO	YES	Theorem 4.23/ Example 4.34

Table 4.2: Table of monotonicity conditions for conditionally strictly positive definite functions of order m on arbitrary spheres

We have here found a broad set of sufficient conditions to verify positive definiteness of different basis functions for both arbitrary dimensions d Tables 4.1 and 4.3 and spheres of fixed dimension Table 4.4. We also gave a new sufficient condition for conditionally positive definite functions of order m on spheres Table 4.2. The additional Examples 4.34 to 4.36 allow us to determine whether those conditions are necessary or sufficient. We believe that the results lead to a better understanding of the connection of the positive definiteness of functions on spheres and their monotonicity properties. So that perhaps in future work we will also be able to give simple necessary and sufficient conditions.

Example 4.34. *The function $\varphi(x) = e^x - 1 = \sum_{k=1}^{\infty} \frac{x^m}{m!}$ is strictly positive definite on $\mathbb{S}^{d-1}$ for arbitrary d according to Theorem 4.17 but it is not absolutely monotone on $[-1,1]$ since $\varphi(x) = e^x - 1 < 0$ for $x \in [-1,0)$ (also the function $\tilde{\phi}(x) = \varphi\left(1 - \frac{x^2}{2}\right)$ is not k-times monotone for any k).*

Example 4.35. *The function $\phi(\theta) = \frac{\pi}{2} - \theta$ is not strictly positive definite on $\mathbb{S}^{d-1}$ for arbitrary d according to Theorem 4.17, because all the coefficients with even indices are*

Function	Monotonicity conditions	Necessary	Sufficient	Proofs/Examples
$\varphi \in C^\infty([-1,1])$, no polynomial	Absolute monotone of order 1 on $[-1,1]$	NO	YES	Theorem 4.23 / Example 4.34
$\phi : [0,\pi] \to \mathbb{R}$, analytic, $\phi''(\pi/2) \neq 0$	Completely monotone of order 1 on $[0,\pi/2]$		YES	Theorem 4.29 /

Table 4.3: Table of monotonicity conditions for strictly positive definite functions of order 1 on arbitrary spheres

Function	Monotonicity conditions	Necessary	Sufficient	Proofs/Examples	Dimension
$\varphi : (-\infty,1] \to \mathbb{R}$, $\widetilde{\phi}(x) = \varphi\left(1-\frac{x^2}{2}\right)$,	$\widetilde{\phi}$ n-times monotone on $[0,\infty)$	NO	YES	Lemma 4.22 / Example 4.34	$n \geq \lfloor \frac{d}{2} \rfloor + 2$
$\phi \in C^{n-2}([0,\infty))$	n-times monotone on $(0,\pi]$	NO	YES	Theorem 4.25 / Example 4.36	$2n \geq d$

Table 4.4: Table of monotonicity conditions for strictly positive definite functions on the sphere $\mathbb{S}^{d-1}$

zero, but it is completely monotone on $[0,\pi/2]$.

Example 4.36. *The function* $\phi(\theta) = 1 - (\theta - \frac{\pi}{2}) + (\theta - \frac{\pi}{2})^2$ *is strictly positive definite on* $\mathbb{S}^{d-1}$ *for arbitrary* d *according to Theorem 4.27, but it is not completely monotone on* $[0,\pi]$ *since* $\phi'(\pi) = \pi - 1 > 0$.

4.3 Shifted surface splines for the sphere

The thin-plate spline (also called surface spline) is defined as

$$\phi(r) = \begin{cases} (-1)^n r^{2m-d} \log(r), & d \text{ even}, \\ (-1)^n r^{2m-d}, & d \text{ odd}, \end{cases} \tag{4.27}$$

$$\text{where } n := \begin{cases} m - \frac{d-2}{2}, & d \text{ even}, \\ m - \frac{d-1}{2}, & d \text{ odd}. \end{cases} \tag{4.28}$$

The function ϕ is conditionally positive definite of order $m - \frac{d-2}{2}$ on $\mathbb{R}^d$ for even dimensions and $m - \frac{d-1}{2}$ for odd dimensions and generally $\lfloor m - \frac{d}{2} + \frac{1}{2} \rfloor$ for all dimensions d, as was described in Example 1.15. The thin-plate splines are well known and frequently used basis functions in $\mathbb{R}^d$. They were introduced as the solution of the following minimisation problem:

$$\text{minimise} \left\{ \|s\|_{H^m(\mathbb{R}^d)} : \; s(\xi) = f(\xi), \forall \xi \in \Xi \right\}, \tag{4.29}$$

where the semi-norm is induced by the linear form

$$\langle f, g \rangle_{H^m(\mathbb{R}^d)} = \sum_{|\alpha|=m} \frac{m!}{\alpha!} \int_{\mathbb{R}^d} D^\alpha f(x) D^\alpha g(x)\, dx.$$

For $m = 2$, which is most frequently used, the norm minimised represents the bending energy of the interpolant. The name therefore refers to a thin metal (or wooden) plate which is fixed in the sites to be interpolated. Duchon was the first to study those functions in two dimensions, they are therefore sometimes referred to as Duchon- or D-splines. The adaptation of the thin-plate spline to the sphere was necessary because of the results of Johnson [Joh98]. He described the so-called boundary effect, which occurs when using Euclidean basis functions interpolation, in cases where the data to be interpolated are only stemming from a closed domain in $\mathbb{R}^d$. He showed that in the case of data being dense in the unit ball, there is a loss of convergence order of the error estimate compared to a set which is dense in $\mathbb{R}^d$.

The result on the convergence order of the thin-plate spline, for dense sets in $\mathbb{R}^d$, as a special case for a grid of the form $\Xi = h\mathbb{Z}^d \subset \mathbb{R}^d$, $h > 0$, were obtained by Buhmann in [Buh90]. He showed that for a function $f \in C^{2m}(\mathbb{R}^d)$, its unique surface spline interpolant s_f in Ξ satisfies

$$\|s_f - f\|_{L^p(\mathbb{R}^d)} = \mathcal{O}(h^{2m}), \quad p \in [1, \infty). \tag{4.30}$$

Johnson showed that for a dense set of points in the unit ball, the convergence order is at most m.

To avoid this boundary effect and to find new error estimates, changes to the basis functions and the methods to derive the error estimates had to be made. We start by describing the surface spline for the sphere which was introduced by Hubbert and Morton, and in the next section we will add a shifted version in analogue to the shifted thin-plate splines in $\mathbb{R}^d$.

4.3.1 Generalised surface splines for the sphere

The idea of an adapted version of the surface splines was first described by Hubbert and Morton in [HM04b] where the generalised surface spline for the sphere $\mathbb{S}^{d-1}$ is defined using

$$\tilde{\phi}(r) = \begin{cases} (-1)^{m-\frac{d-3}{2}} r^{2m-(d-1)} \log(r), & d \text{ odd}, \\ (-1)^{m-\frac{d-2}{2}} r^{2m-(d-1)}, & d \text{ even}, \end{cases} \tag{4.31}$$

taking into account that the sphere is only a $(d-1)$-dimensional manifold. If we now replace the Euclidean distance by the geodesic distance we get, by applying $\|\xi - \nu\| = \sqrt{2 - 2\xi^T \nu}$ and $t = \xi^T \nu$,

$$\varphi(x) = \begin{cases} (-1)^{m-\frac{d-3}{2}} (2-2x)^{m-(d-1)/2} \log(2-2x), & d \text{ odd}, \\ (-1)^{m-\frac{d-2}{2}} (2-2x)^{m-(d-1)/2}, & d \text{ even}. \end{cases} \tag{4.32}$$

If we wanted to include the standard geodesic distance, our function would have to depend on $d(\xi, \nu) = \arccos(\xi^T \nu)$ but in this case it is easier to use $x = \xi^T \nu$ instead.

To be able to give error estimates for the interpolation using spherical basis functions we want to use the global error bound by Hubbert, cited as Theorem 4.16, if possible. In order to do this, we need to compute the Fourier decay (defined in Definition 4.11) of the Fourier coefficients (defined in (4.7)) of the basis function.

For the generalised surface spline the rate of α-decay was determined by Hubbert and Morton, who proved the Fourier coefficients of the function to be as follows:

Theorem 4.37 ([HM04a], Lemma 3)**.** *For even values of d the Fourier coefficients of φ have the form:*

$$\hat{\varphi}(k) = \frac{2^{2m} \pi^{\frac{d-3}{2}} \Gamma(k + \frac{d-1}{2} - m) \Gamma(m - \frac{d-1}{2} + 1) \Gamma(m)}{\Gamma(m + k + \frac{d-1}{2})}, \tag{4.33}$$

and for d odd

$$\hat{\varphi}(k) = \frac{2^{2m-1}\pi^{\frac{d-1}{2}}\Gamma(k+\frac{d-1}{2}-m)\Gamma(m-\frac{d-1}{2}+1)\Gamma(m)}{\Gamma(m+k+\frac{d-1}{2})}. \tag{4.34}$$

Therefore the surface spline has α-Fourier decay with $\alpha = 2m-(d-1)$.

The great similarities between the d-dimensional Fourier transform of the thin-plate spline computed in Example 3.17 and the Fourier coefficients are no coincidence, but a result of Proposition 4.9. From the above results an error estimate is easily derived, using what we cited as Theorem 4.16, we cite it without proof.

Theorem 4.38 ([HM04a], Theorem 4)**.** *Let $m,\ d \in \mathbb{N}$ be such that $m > \frac{d-1}{2}$. Let $f \in W_2^{2m}(\mathbb{S}^{d-1})$ and s_f denote the unique φ-based interpolant, where φ is as in* (4.32)*, to f over a set $\Xi \subset \mathbb{S}^{d-1}$ of distinct data points with mesh-norm h. Then we have*

$$\|s_f - f\|_{L^p(\mathbb{S}^{d-1})} = \begin{cases} \mathcal{O}\left(h^{2m-\frac{d-1}{2}+\frac{d-1}{p}}\right), & p \in [2,\infty]; \\ \mathcal{O}\left(h^{2m}\right), & p \in [1,2]. \end{cases} \tag{4.35}$$

The shifted surface spline for the sphere

We now turn to the shifted version of the surface spline and compute the corresponding Fourier coefficients and rate of decay. This basis function has to our knowledge not been considered on the sphere.

We start by defining the generalised shifted surface spline for the sphere, which is a shifted version of (4.32),

$$\varphi_c(t) = \begin{cases} (-1)^{m-\frac{d-3}{2}}(2-2t+c^2)^{m-(d-1)/2}\log(2-2t+c^2), & d \text{ odd}, \\ (-1)^{m-\frac{d-2}{2}}(2-2t+c^2)^{m-(d-1)/2}, & d \text{ even}, \end{cases} \tag{4.36}$$

where $m \geq \frac{d-1}{2}$ and $c \in \mathbb{R}$ is a smoothing parameter which can be used to adjust the basis function to different data distributions and target functions. The influence of the smoothing parameter on stability and accuracy of surface spline interpolation is studied numerically in Section 5.1. We note here that in the case of d even the function is equal to a generalised spherical multiquadric. We first apply a theorem by Castell and Filbir [zCF04] which is derived from Proposition 4.9.

Theorem 4.39 ([zCF04]). *If for some $0 < \gamma < d$ the generalised Fourier transform of a radial function Φ, which is positive definite of order $k \in \mathbb{N}$, satisfies*

$$\widehat{\Phi}(t) = \mathcal{O}(t^{-2k-\gamma}), \quad \text{as } t \to 0,$$

then the coefficients $\hat{\varphi}(j)$ in the zonal series expansion satisfy

$$|\hat{\varphi}(j)| = \mathcal{O}(j^{-2k-\gamma+1}), \quad \text{as } j \to \infty.$$

Lemma 4.40. *The Fourier coefficients of the shifted surface spline φ_c for the sphere (as defined in eq.* (4.32)*) satisfy*

$$\hat{\varphi}(j) = \mathcal{O}(j^{-2m}), \quad j \to \infty.$$

Proof. The shifted surface spline for the sphere is the restriction to the sphere of the Euclidean basis function

$$\phi_c(r) = \begin{cases} (-1)^{m-\frac{d-3}{2}}(r^2+c^2)^{m-(d-1)/2}\log(r^2+c^2), & d \text{ odd}, \\ (-1)^{m-\frac{d-2}{2}}(r^2+c^2)^{m-(d-1)/2}, & d \text{ even}. \end{cases} \tag{4.37}$$

The generalised Fourier transform of the shifted surface spline was computed in Example 3.17 and the generalised Fourier transform of the multiquadric was computed in Example 3.15, they are given by

$$\widehat{\Phi_c}(t) = \begin{cases} 2^{m-\frac{d-3}{2}}\left(\frac{c}{t}\right)^{m+\frac{1}{2}} K_{m+\frac{1}{2}}(ct), & d \text{ odd}, \\ \frac{(-1)^{m-\frac{d-2}{2}}2^{m-\frac{d-3}{2}}}{\Gamma\left(-m+\frac{d-1}{2}\right)}\left(\frac{c}{t}\right)^{m+\frac{1}{2}} K_{m+\frac{1}{2}}(ct), & d \text{ even}. \end{cases} \tag{4.38}$$

Using [AS72] (9.6.9)

$$K_\nu(z) \sim \frac{1}{2}\Gamma(\nu)\left(\frac{1}{2}z\right)^{-\nu}, \quad \text{for } z \to 0,$$

we deduce that

$$|\widehat{\Phi_c}(t)| = \mathcal{O}(t^{-2m-1}), \quad t \to 0,$$

and we can apply Theorem 4.39 and determine that the Fourier coefficients will decay like $\hat{\varphi}(j) = \mathcal{O}(j^{-2m})$. $\square$

The result above is not enough to be applied to the mentioned error estimates. Until now we only have a lower bound on the decay of the coefficients. We now compute the Fourier coefficients to be able to determine the order of α-Fourier decay and to characterise the function.

Theorem 4.41. *The Fourier coefficients of the shifted surface spline defined in* (4.36) *are given for $j > m - \frac{d-1}{2}$ and odd d by:*

$$\hat{\varphi}_c(j) = 2^{2m-1}\omega_{d-1}\Gamma\left(\frac{d-1}{2}\right)\Gamma\left(m-\frac{d-3}{2}\right)\left(\frac{4}{4+c^2}\right)^{j-m+\frac{d-1}{2}} \cdot \frac{\Gamma\left(j+\frac{d-1}{2}\right)\Gamma\left(j-m+\frac{d-1}{2}\right)}{\Gamma\left(2\left(j+\frac{d-1}{2}\right)\right)}F\left(j-m+\frac{d-1}{2}; j+\frac{d-1}{2}; 2\left(j+\frac{d-1}{2}\right); \frac{4}{4+c^2}\right). \tag{4.39}$$

For even d the Fourier coefficients are given by:

$$\hat{\varphi}_c(j) = 2^{2m-3}\omega_{d-1}\Gamma\left(\frac{d-1}{2}\right)\Gamma\left(m-\frac{d-3}{2}\right)\left(\frac{4}{4+c^2}\right)^{j-m+\frac{d-1}{2}} \cdot \frac{(-1)^{j+m-\frac{d-2}{2}}\Gamma\left(j+\frac{d-1}{2}\right)}{\Gamma\left(2\left(j+\frac{d-1}{2}\right)\right)\Gamma(m-\frac{d-3}{2}-j)}F\left(j-m+\frac{d-1}{2}; j+\frac{d-1}{2}; 2\left(j+\frac{d-1}{2}\right); \frac{4}{4+c^2}\right). \tag{4.40}$$

Proof. We follow the scheme introduced in [HM04a] for the non-shifted version. To do so we use the connection

$$\tilde{\varphi}_c(t) = (-1)^{m-\frac{d-3}{2}}\frac{\partial}{\partial\beta}(2-2t+c^2)^{\beta}\ |_{\beta=m-\frac{d-1}{2}}\ . \tag{4.41}$$

This can be applied to Fourier coefficients as well, since

$$(2-2\xi^T\nu+c^2)^{\beta} = \sum_{j=0}^{\infty} a_j(\beta,d)\sum_{\ell=0}^{N_{j,d}} Y_{j,\ell}(\xi)Y_{j,\ell}(\nu)$$

with

$$a_j(\beta,d) = \omega_{d-1}\int_{-1}^{1}(2-2t+c^2)^{\beta}P_{j,d}(t)(1-t^2)^{\frac{d-3}{2}}\,dt.$$

Therefore the Fourier coefficients of φ_c satisfy:

$$\hat{\varphi}_c(j) = \frac{\partial}{\partial\beta}a_j(\beta,d)|_{\beta=m-\frac{d-1}{2}}.$$

We first need to compute $a_j(\beta, d)$. Those are the Fourier coefficients of the multiquadric which have (in the slightly different form $a_j = \frac{a_j(\beta,d)N_{j,d}}{\omega_d}$) already been computed by Baxter and Hubbert in [HB01], we nevertheless include the computation to give a self-contained proof of our result. We start by inserting the Rodrigues' formula of the d-dimensional Legendre polynomial of order j:

$$a_j(\beta, d) = \underbrace{\frac{\omega_{d-1}(-1)^j\Gamma\left(\frac{d-1}{2}\right)}{2^j\Gamma\left(j+\frac{d-1}{2}\right)}}_{c_{j,d}} \int_{-1}^{1} (2-2t+c^2)^\beta \frac{\partial^j}{\partial t^j}(1-t^2)^{j+\frac{(d-3)}{2}}\, dt.$$

Using integration by parts j-times we get

$$\begin{aligned} a_j(\beta, d) =& c_{j,d}(-1)^j \int_{-1}^{1} \left(\frac{\partial^j}{\partial t^j}(2-2t+c^2)^\beta\right)(1-t^2)^{\frac{j+(d-3)}{2}}\, dt \\ =& c_{j,d}\frac{\Gamma(\beta+1)2^j}{\Gamma(\beta+1-j)} \int_{-1}^{1} (2-2t+c^2)^{\beta-j}(1-t^2)^{j+\frac{(d-3)}{2}}\, dt \\ =& c_{j,d}\frac{\Gamma(\beta+1)2^\beta}{\Gamma(\beta+1-j)} \int_{-1}^{1} \left(1+\frac{c^2}{2}-t\right)^{\beta-j}(1-t)^{j+\frac{(d-3)}{2}}(1+t)^{j+\frac{(d-3)}{2}}\, dt. \end{aligned}$$

Now we substitute $t = 2u - 1$ and derive

$$\begin{aligned} a_j(\beta, d) =& c_{j,d}\frac{\Gamma(\beta+1)2^{\beta+1}}{\Gamma(\beta+1-j)} \int_{0}^{1} \left(2+\frac{c^2}{2}-2u\right)^{\beta-j}(2-2u)^{j+\frac{(d-3)}{2}}(2u)^{j+\frac{(d-3)}{2}}\, du \\ =& c_{j,d}\frac{\Gamma(\beta+1)2^{2\beta+j+d-2}}{\Gamma(\beta+1-j)\left(\frac{4+c^2}{4}\right)^{-\beta+j}} \int_{0}^{1} \left(1-\frac{4}{4+c^2}u\right)^{\beta-j}(1-u)^{j+\frac{(d-3)}{2}}u^{j+\frac{(d-3)}{2}}\, du. \end{aligned}$$

This can be transformed into a hypergeometric function using ([AS72], 15.3.1)

$$\begin{aligned} a_j(\beta, d) = c_{j,d}&\frac{\Gamma(\beta+1)2^{2\beta+j+d-2}\left(\frac{4+c^2}{4}\right)^{\beta-j}}{\Gamma(\beta+1-j)}\frac{\Gamma\left(j+\frac{d-1}{2}\right)^2}{\Gamma\left(2j+d-1\right)} \\ &F\left(j-\beta; j+\frac{d-1}{2}; 2\left(j+\frac{d-1}{2}\right); \frac{4}{4+c^2}\right) \end{aligned}$$

where $F(a, b; \underline{c}; z)$ is the hypergeometric function ([AS72], 15.1.1) defined by

$$F(a, b; \underline{c}; z) = \frac{\Gamma(\underline{c})}{\Gamma(a)\Gamma(b)} \sum_{k=0}^{\infty} \frac{\Gamma(a+k)\Gamma(b+k)}{\Gamma(\underline{c}+k)}\frac{z^k}{k!}. \tag{4.42}$$

We sort those terms in a way suitable for determining the derivative with respect to β:

$$a_j(\beta,d)=\alpha_j(\beta,d)\underbrace{\left(\frac{4+c^2}{4}\right)^{\beta-j}2^{d-2+2\beta}F\left(j-\beta,j+\frac{d-1}{2},2\left(j+\frac{d-1}{2}\right);\frac{4}{4+c^2}\right)}_{=:u(\beta)},\tag{4.43}$$

where

$$\alpha_j(\beta,d)=\underbrace{\frac{\omega_{d-1}(-1)^j\Gamma\left(\frac{d-1}{2}\right)\Gamma\left(j+\frac{d-1}{2}\right)}{\Gamma\left(2\left(j+\frac{d-1}{2}\right)\right)}}_{:=c_j}\underbrace{\frac{\Gamma(\beta+1)}{\Gamma(\beta-j+1)}}_{=:h(\beta)}.\tag{4.44}$$

The series in (4.42) with $a=j-\beta$, $b=j+\frac{d-1}{2}$, $\underline{c}=2\left(j+\frac{d-1}{2}\right)$, is absolutely convergent for $|z|\le 1$ and $-d/2<\beta$. So for the Fourier coefficients of the shifted surface spline we get

$$\begin{aligned}(-1)^{-m+\frac{d-3}{2}}\hat{\varphi}_c(j)=&\quad\frac{\partial}{\partial\beta}a_j(\beta,d)\mid_{\beta=m-\frac{d-1}{2}}\\ =&\quad\frac{\partial}{\partial\beta}\left(c_jh(\beta)u(\beta)\right)\mid_{\beta=m-\frac{d-1}{2}}\\ =&\quad c_j\left(h'(\beta)u(\beta)+h(\beta)u'(\beta)\right)\mid_{\beta=m-\frac{d-1}{2}},\end{aligned}$$

where $h(\beta)=\frac{\Gamma(\beta+1)}{\Gamma(\beta-j+1)}=\beta(\beta-1)\cdots(\beta-j+1)=0$ for all $j>\beta$ if $\beta\in\mathbb{N}_0$. And with

$$\frac{\partial}{\partial\beta}h(\beta)=\sum_{i=0}^{j-1}\prod_{\substack{k=0\\k\neq i}}^{j-1}(\beta-k),$$

we can deduce for $\beta=m-\frac{d-1}{2}$ and $j>m-\frac{d-1}{2}$:

$$h'\left(m-\frac{d-1}{2}\right)=(-1)^{j-m+\frac{d-3}{2}}\Gamma\left(m-\frac{d-1}{2}+1\right)\Gamma\left(j-m+\frac{d-1}{2}\right).$$

The combination gives us, for $j>m-\frac{d-1}{2}$,

$$\begin{aligned}\hat{\varphi}_c(j)=&\frac{\omega_{d-1}\Gamma\left(\frac{d-1}{2}\right)\Gamma\left(j+\frac{d-1}{2}\right)\Gamma\left(m-\frac{d-1}{2}+1\right)\Gamma\left(j-m+\frac{d-1}{2}\right)}{\Gamma\left(2\left(j+\frac{d-1}{2}\right)\right)}\left(2+\frac{c^2}{2}\right)^{m-\frac{d-1}{2}-j}\\ &2^{j+m+\frac{d-1}{2}}F\left(j-m+\frac{d-1}{2},j+\frac{d-1}{2};2(j+\frac{d-1}{2});\frac{4}{4+c^2}\right).\end{aligned}$$

For the case d even the coefficients are a special case of the ones computed in (4.43), to be precise

$$\hat{\varphi}(j) = (-1)^{m-\frac{d-2}{2}} a_j\left(m - \frac{d-1}{2}, d\right).$$

$\square$

We now determine the decay rate of these newly computed Fourier coefficients. We know that for the hypergeometric function (4.42)

$$F(a, b; \underline{c}; z) \leq F(a, b; \underline{c}; 1)$$

holds for all $a, b, \underline{c} \in \mathbb{N}$ and $0 < z < 1$, $z \in \mathbb{R}$. From this we can easily deduce for all $j \geq m - \frac{d-1}{2}$ and with $C \in \mathbb{R}_{>0}$ a parameter independent of j which can change from one appearance to another

$$\begin{aligned} 0 \leq \hat{\varphi}_c(j) &\leq C \frac{\Gamma\left(j + \frac{d-1}{2}\right)\Gamma\left(j - m + \frac{d-1}{2}\right)\left(\frac{4}{4+c^2}\right)^j}{\Gamma\left(2\left(j + \frac{d-1}{2}\right)\right)} \\ &\quad \cdot F\left(j - m + \frac{d-1}{2}, j + \frac{d-1}{2}; 2\left(j + \frac{d-1}{2}\right); 1\right) \\ &\overset{[AS72](15.1.20)}{=} C \frac{\Gamma\left(j - m + \frac{d-1}{2}\right)\left(\frac{4}{4+c^2}\right)^j}{\Gamma\left(j + m + \frac{d-1}{2}\right)} = \mathcal{O}\left(\frac{\alpha^j}{j^{2m}}\right), \quad \text{for } d \text{ odd}, \end{aligned}$$

where $\alpha = \frac{4}{4+c^2}$. The above equation shows that we will only be able to determine an α-decay rate if the parameter $c = 0$. For $c \neq 0$ the Fourier coefficients decay exponentially fast.

For the generalised multiquadric (or the shifted surface spline in even dimensions) a similar result can be deduced for $j \geq m - \frac{d-1}{2}$, i.e.

$$\begin{aligned} 0 \leq \hat{\varphi}_c(j) &\leq C \frac{\left(\frac{4}{4+c^2}\right)^{j-m+\frac{d-1}{2}}(-1)^{j+m-\frac{d-2}{2}}\Gamma\left(j + \frac{d-1}{2}\right)}{\Gamma\left(2\left(j + \frac{d-1}{2}\right)\right)\Gamma(m - \frac{d-3}{2} - j)} \\ &\quad \cdot F\left(j - m + \frac{d-1}{2}; j + \frac{d-1}{2}; 2\left(j + \frac{d-1}{2}\right); 1\right) \\ &\underset{([AS72]15.1.20)}{=} C\left(\frac{4}{4+c^2}\right)^{j-m+\frac{d-1}{2}} \frac{(-1)^{j+m-\frac{d-2}{2}}}{\Gamma\left(m - \frac{d-3}{2} - j\right)\Gamma\left(j + \frac{d-1}{2} + m\right)}, \end{aligned}$$

an estimate can be computed using the reflection formula for the Γ function ([AS72], (6.1.17)) with $z = m - \frac{d-3}{2} - j$:

$$\Gamma\left(m - \frac{d-3}{2} - j\right)\Gamma\left(-m + \frac{d-1}{2} + j\right) = \frac{\pi}{\sin(\pi z)} = \pi(-1)^{j-m+\frac{d-2}{2}}.$$

This yields

$$\hat{\varphi}_c(j) \leq C\left(\frac{4}{4+c^2}\right)^{j-m+\frac{d-1}{2}} \frac{\Gamma(-m+\frac{d-1}{2}+j)}{\pi\Gamma\left(j+\frac{d-1}{2}+m\right)} = \mathcal{O}\left(\frac{\alpha^j}{j^{2m}}\right),$$

showing that the generalised multiquadric has faster than exponentially decaying Fourier coefficients for all $c \neq 0$.

Even though those results do not allow us to give new error results, we can easily see that the shifted versions are conditionally positive definite of order $m - \frac{d-1}{2}$ for d odd and $m - \frac{d-2}{2}$ for d even. The results of [Hub02] suggest that functions with exponential Fourier decay produce smaller interpolation errors when the target function is sufficiently smooth. Also the famous paper 'Scattered Data Interpolation: Tests of some Methods' by Franke [Fra82] showed that for interpolation in $\mathbb{R}^d$ the multiquadric and the thin-plate spline performed better than other basis functions and other interpolation techniques.

Therefore we will study in the next chapter the performance of the shifted surface spline interpolation on $\mathbb{S}^2$ while also evaluating the stability of the method.

4.4 Shifts and scaling of spherical basis functions

Motivated by the shifted surface spline and the results of Section 3.2 for Euclidean spaces, we study shifts of spherical basis functions. The shifts which we now introduce are slightly different from the Euclidean one. We start by shifts of basis functions in the form $\varphi : [-1,1] \to \mathbb{R}$.

A shift of such a function will require our knowledge of an extension of such a function to either $[-1-c, 1]$ or $(-1, 1+c]$ but we will see that this extension usually is known. We define

$$\psi(\tau, x) := \varphi(x+\tau),$$

where φ is defined on the interval $[-1-\tau, 1+\tau] \cup [-1,1]$. If φ is the restriction of a Euclidean basis function $\phi : \mathbb{R}_{\geq 0} \to \mathbb{R}$ to the sphere, we know that $\varphi(x) := \phi(\sqrt{2-2x})$. We can now identify the newly defined spherical shift with the one defined in Chapter 3.2:

$$\begin{aligned} &\phi_c(r) = \phi(\sqrt{r^2+c^2}) \\ \to \phi(\sqrt{2-2x+c^2}) =&\phi\left(\sqrt{2-2\left(x-\frac{c^2}{2}\right)}\right) = \varphi\left(x-\frac{c^2}{2}\right) = \psi\left(-\frac{c^2}{2}, x\right). \end{aligned}$$

We can thereby deduce using the results of Section 4.2.

Lemma 4.42. 1. *For all $\varphi \in C((-\infty, 1])$ which are absolutely monotone of order m on $(-\infty, 1)$ (meaning $\varphi^{(m)}$ is absolutely monotone on $(-\infty,1)$), the function $\psi(\tau, \cos(\cdot))$, $\tau < 0$, is conditionally strictly positive definite of order m on $\mathbb{S}^{d-1}$ for all $d \geq 2$.*

2. *Let $\varphi \in C^\infty([-1+\tau, 1+\tau] \cup [-1,1])$ be absolutely monotone of order m on $x \in [-1+\tau, 1+\tau] \cup [-1,1]$ and let it be no polynomial. Then the function $\psi(\tau, \cos(\cdot))$ is conditionally strictly positive definite of order m on $\mathbb{S}^{d-1}$ for all $d \geq 3$.*

Proof. The lemma follows directly from Theorem 4.18 and Theorem 4.23. □

We can further use Schoenberg's representation of positive definite spherical functions to derive another interesting result.

Theorem 4.43. *Let $\varphi(x) = \sum_{k=0}^\infty a_k x^k$, $a_k \geq 0$, $k \geq m$, $\sum_{k=0}^\infty a_k (1+\tau)^k < \infty$ and $a_k > 0$ for infinitely many k. Then $\psi(\tau, \cos(\cdot))$ is conditionally strictly positive definite of order m on $\mathbb{S}^{d-1}$ for $\tau > 0$ and arbitrary $d \geq 2$.*

Proof. We can express $\psi(\tau,\cdot)$ in the form

$$\varphi(x+\tau) = \sum_{k=0}^{\infty} a_k (x+\tau)^k = \sum_{k=0}^{\infty} a_k \sum_{j=0}^{k} \binom{k}{j} x^j \tau^{k-j} = \sum_{n=0}^{\infty} b_n x^n,$$

where $b_n > 0$, as a sum of positive coefficients. Now $\psi(\tau,\cdot)$ is conditionally strictly positive definite of order m as a consequence of Lemma 4.24. □

What should be noted about this theorem is, that the function φ itself does not need to be strictly positive definite of order m. We will illustrate this by giving some examples.

Example 4.44. *The secans*

$$\sec(z) = \frac{1}{\cos(z)}, \quad z \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right),$$

has the series expansion ([AS72], (4.3.69))

$$\sec(z) = \sum_{n=0}^{\infty} \frac{(-1)^n E_{2n}}{(2n)!} z^{2n}, \quad |z| < \frac{\pi}{2}.$$

For the Euler numbers E_n we find (23.1.15)

$$0 < (-1)^n E_{2n} \leq \infty.$$

The last theorem now allows us to deduce that $\sec(t+\tau)$ *for* $1 - \frac{\pi}{2} > \tau > 0$ *is strictly positive definite in arbitrary dimensions.*

In the supplementary material to the paper 'Strictly positive definite functions on spheres' [Gne13] Gneiting stated 18 open problems on strictly positive definite functions on spheres. Problem 8 is about scaling spherical basis functions $\phi : [0,\pi] \to \mathbb{R}$ in the way

$$\widetilde{\phi}(\cdot) = \phi\left(\frac{\cdot}{\alpha}\right), \quad \alpha > 0.$$

For Euclidean basis function scaling of this form is always possible because the effect of scaling is equivalent to projecting a given set of points to a set where all points have α-times their original distance. Since the function is positive definite for arbitrary point distributions, scaling preserves positive definiteness.

For the sphere we cannot expect similar results even though scaling of the described form is possible for all the spherical basis functions derived in Section 4.2. This is because we defined positive definiteness using monotonicity properties and those are preserved by scaling, even though we have to restrict ourself to the case $\alpha > 1$ if the basis function is only known on $[0, \pi]$.

For spherical basis functions which are only positive definite on $\mathbb{S}^{d-1}$ up to some dimension d we do not know if a scaled basis function exists. We can not solve the problem stated by Gneiting but we suggest a smoothing variable which is applicable to such functions, even though we can not preserve the dimension of positive definiteness entirely.

Lemma 4.45. *Let $\varphi : [-1, 1] \to \mathbb{R}$ be strictly positive definite on $\mathbb{S}^{d-1}$, then the scaled function*

$$\widetilde{\varphi}(\cdot) = \varphi\left((1 - \alpha^2) \cdot + \alpha^2\right), \quad \alpha \in (0, 1),$$

is strictly positive definite on $\mathbb{S}^{d-2}$.

Proof. Let $\Xi \subset \mathbb{S}^{d-2}$ be any finite set of distinct points. Then

$$\Xi_{\sqrt{1-\alpha^2}} = \left\{\sqrt{1 - \alpha^2} \cdot \xi |\ \xi \in \Xi\right\}$$

is a subset of the sphere of radius $\sqrt{1 - \alpha^2}$, denote by $\mathbb{S}^{d-2}_{\sqrt{1-\alpha^2}}$. This sphere can be embedded in the unit sphere $\mathbb{S}^{d-1}$. We define the set $\widetilde{\Xi} = \left\{(\xi^T, \alpha) |\ \xi \in \Xi_{\sqrt{1-\alpha^2}}\right\}$. Since φ is positive definite on $\mathbb{S}^{d-1}$ we know that

$$\sum_{\tilde{\xi}, \tilde{\nu} \in \widetilde{\Xi}} \lambda_{\tilde{\xi}} \varphi\left(\tilde{\xi}^T \tilde{\nu}\right) \lambda_{\tilde{\nu}} > 0, \quad \forall \lambda \in \mathbb{R}^{|\widetilde{\Xi}|},$$

unless $\lambda \equiv 0$. From the definition of the set $\widetilde{\Xi}$ we deduce

$$\sum_{\tilde{\xi}, \tilde{\nu} \in \widetilde{\Xi}} \lambda_{\tilde{\xi}} \varphi\left(\tilde{\xi}^T \tilde{\nu}\right) \lambda_{\tilde{\nu}} = \sum_{\xi, \nu \in \Xi} \lambda_{\tilde{\xi}} \varphi\left((1 - \alpha^2) \xi^T \nu + \alpha^2\right) \lambda_{\tilde{\nu}}$$

which proves the lemma. ∎

Chapter 5

Numerical Evaluation

5.1 Test of some spherical basis functions

Our goal is to compare the performance of the new spherical basis functions introduced in the last chapter to some well known basis functions, as for example the Gaussian or the multiquadric. The basis functions we include in our numerical evaluation are therefor

$$\varphi_1(x) = (2-2x)\log(2-2x), \text{ the surface spline,} \tag{TPS}$$

$$\varphi_2(x) = (2-2x+c^2)\log(2-2x+c^2),\ c>0, \text{ shifted surface spline,} \tag{STPS}$$

$$\varphi_3(x) = e^{-\alpha(2-2x)},\ \alpha>0, \text{ Gaussian,} \tag{GAU}$$

$$\varphi_4(x) = \sqrt{c^2+2-2x}, c>0, \text{ multiquadric,} \tag{MQ}$$

$$\varphi_5(x) = \frac{1}{2-2x+c^2},\ c>0, \text{ spherical reciprocal multiquadric,} \tag{IMQ}$$

$$\varphi_6(x) = -\frac{1}{\pi}\left(\frac{\pi}{2}+\arccos(x)\right)^{1/2},\ \text{ new s.b.f from Example 4.31,} \tag{SRT}$$

$$\varphi_7(x) = If_4(x) = \int_{-1}^{x}(t-\arccos(\theta))_+^4\,d\theta,\ \text{ compactly supported s.b.f. from [BzC17]} \tag{CSBF}$$

$$\varphi_8(x) = \frac{1}{\cos(x+c)},\ c>0, \text{ shifted secans.} \tag{SEC}$$

The only error estimates we can use to give a prognosis of the performance are the ones by Hubbert we cited in Theorem 4.15. These are only applicable is the decay rate of the Fourier coefficients of the basis function is known and not exponential. The coefficients of the surface spline have α-Fourier decay; the decay rate of the coefficients of the shifted surface spline is exponential but dependent on the shift parameter c and the Gaussian also has exponentially decaying Fourier coefficients. Therefore we can give no prognosis of the error for most of the studied functions.

The numerical results presented in [Hub02] suggest that basis functions with α-Fourier decay produce larger errors but the stability is higher than for functions with exponentially fast decaying coefficients. We want to see if we can reproduce these results with the newly introduced basis functions. A topic of special interest is, how, depending on the choice of c the shifted surface spline performs in comparison. Thus we start by studying the stability and accuracy of the shifted surface spline before we proceed with the overall comparison.

5.1.1 The shifted surface spline on $\mathbb{S}^2$

We first investigate the error of the shifted surface spline interpolation depending on the parameter c. The test functions to be approximated are, for $\xi = (\xi_1, \xi_2, \xi_3)^T \in \mathbb{S}^2$,

$$f_1(\xi) = \sin(\xi_1)\sin(\xi_2)\sin(\xi_3), \tag{5.1}$$

$$f_2(\xi) = \frac{25}{25 + (\xi_1 - 0.2)^2 + 2\xi_2 + \xi_3}, \tag{5.2}$$

$$f_3(\xi) = e^{\xi_1^2}. \tag{5.3}$$

We decided on the first test function because it has already been used as a test function for spherical basis functions (for example in [Hub02]) thus it gives us comparability to other studies. We decided on the second because of its singularity, which is not on the surface of the sphere and chose in addition the third test function because it is radially symmetric. The interpolation points are computed using the procedure described in Appendix B the aim of the procedure is to generate a near-uniformly distributed set. The error estimates for the L^∞ and L^2 error are computed from a set Θ, approx. 10000 points, also distributed using the same algorithm. The errors are approximated by

$$\|s - f\|_{L^p}^p \approx \frac{\sum_{\xi \in \Theta} |s(\xi) - f(\xi)|^p}{|\Theta|}, \tag{5.4}$$

$$\|s - f\|_{L^\infty} \approx \max_{\xi \in \Theta} |s(\xi) - f(\xi)|. \tag{5.5}$$

We computed the errors for 10.000 values of c. We found that in our test the error decreases with bigger c, the effect seems only to stop at some c because the condition number of the interpolation matrix gets too big for computation. The results are displayed in Figure 5.1. The effect we see was also described in [Hof13], but for thin-plate

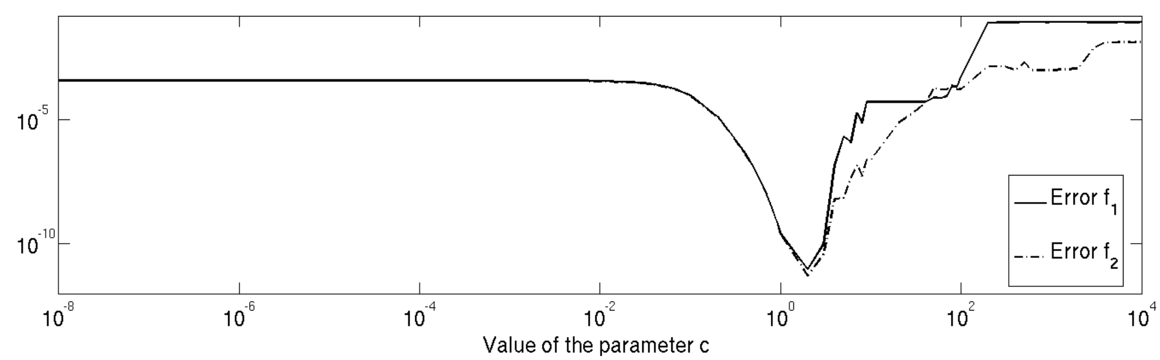

Figure 5.1: Error depending on c when interpolating f_1 and f_2 using φ_2 and approx. 256 points

splines in Euclidean spaces.

From the results we further deduct that the region $c = 10^{-2}$ to $c = 1000$ is the most interesting one for practical applications because there is a significant error reduction. The L^2 error estimate is once more given for different numbers of points and different test functions in Figure 5.2. The results of the computation show that the optimal choice of c depends on the number of points. It also is dependent on the function to be interpolated but the influence of this factor seems significantly smaller than the dependency on the number of points. We believe that the decrease of the error for increasing values of c is due to the increasing flatness of the shifted surface spline. Similar results were reported in [Mon11] for choosing shape parameters of basis functions in $\mathbb{R}^d$.

Convergence of the error compared to the surface spline with $c = 0$

We know from Theorem 4.16, together with the results of Section 4.3.1, that the decay of the L^2 error of surface spline interpolation is $\mathcal{O}(h^4)$, when $h \to 0$ on $\mathbb{S}^2$ and $m = 2$. Our results in Section 4.3.1 show that for positive values of c, the decay rate of the Fourier coefficients is exponential. We want to see if we can find an increase in the rate of decay of the error. To do so, we compute an estimate of the approximation order k_p by

$$\frac{E_{p,n}}{E_{p,2n}} \approx \left(\frac{h_n}{h_{2n}}\right)^{k_p},$$

where $E_{p,n}$ is our approximation of the L^p error, when performing interpolation with approx. n points as described in (5.4) and (5.5). The factor h_n/h_{2n} can, for the set of data points (describe in Appendix B), be approximated by $\sqrt{2}$. The results are shown for the surface spline with $c = 0$ and $c = 1$ in Table 5.1 and 5.2. For $c = 0$ we can

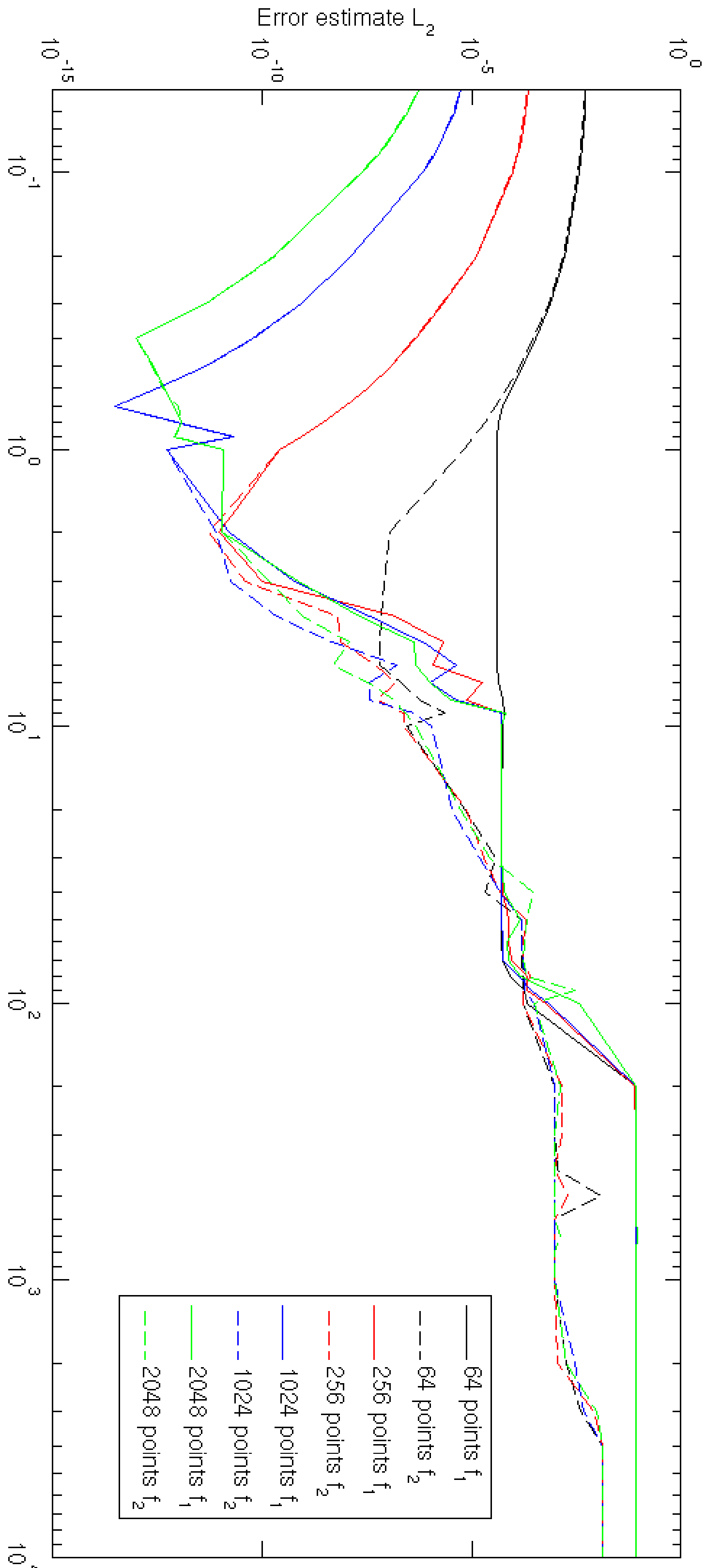

Figure 5.2: Error depending on c when interpolating f_1 and f_2 using φ_1

Points	Error L^∞	Error L^2	k_∞	k_2
n=16	$1.9763 \cdot 10^{-1}$	$7.6197 \cdot 10^{-2}$	$\star$	$\star$
n=32	$7.0067 \cdot 10^{-2}$	$2.6806 \cdot 10^{-2}$	2.9920	3.0144
n=64	$1.6240 \cdot 10^{-2}$	$6.1337 \cdot 10^{-3}$	4.2184	4.2554
n=128	$3.6942 \cdot 10^{-3}$	$1.4671 \cdot 10^{-3}$	4.2725	4.1276
n=256	$9.6536 \cdot 10^{-4}$	$3.7641 \cdot 10^{-4}$	3.8722	3.9252
n=512	$2.2820 \cdot 10^{-4}$	$8.9823 \cdot 10^{-5}$	4.1616	4.1343
n=1024	$5.8714 \cdot 10^{-5}$	$2.3142 \cdot 10^{-5}$	3.9170	3.9131

Table 5.1: Estimate of the convergence order of the surface spline φ_1

Points	Error L^∞	Error L^2	k_∞	k_2
n=16	$2.0389 \cdot 10^{-2}$	$5.3206 \cdot 10^{-3}$	$\star$	$\star$
n=32	$1.0903 \cdot 10^{-3}$	$3.9958 \cdot 10^{-4}$	8.4499	7.4701
n=64	$1.4973 \cdot 10^{-4}$	$3.9306 \cdot 10^{-5}$	5.7287	6.6913
n=128	$4.1203 \cdot 10^{-7}$	$8.9277 \cdot 10^{-8}$	17.0112	17.5640
n=256	$1.5982 \cdot 10^{-9}$	$2.5184 \cdot 10^{-10}$	16.0200	16.9390
n=512	$8.9110 \cdot 10^{-13}$	$1.4347 \cdot 10^{-13}$	21.6170	21.5555
n=1024	$3.5083 \cdot 10^{-12}$	$5.2694 \cdot 10^{-13}$	-3.9542	-3.7537

Table 5.2: Estimate of the convergence order of the shifted surface spline φ_2 with $c = 1$

reproduce the expected decay rate of $k = 4$. For $c = 1$ we see that there seems to be no upper bound to the order. The process stops at 1024 points probably because of the ill conditioning of the interpolation matrix.

Optimal choice of the parameter c

To find a connection between the mesh-distance of our point set and the optimal choice of c we compute approximately optimal choices of c for a bigger variety of point numbers. Our test set is still derived using the method described in Appendix B, for this point set on the sphere we can approximate the mesh distance with $h \approx \sqrt{\frac{2\cdot\pi}{n}}$. In Table 5.3 we choose c to minimise the resulting L^∞ or L^2 error, but by displaying the condition numbers of the resulting interpolation matrices, we see that this choice is not optimal. Since the condition number gets too big for computation to be considered stable.

Therefore we either set a maximum to the condition number, which then will make us choose the optimal c with condition smaller than this maximum. Or we can apply preconditioning techniques to the matrix or the basis function. For example we could form a more stable set of basis functions from the same space of basis functions as described in [BLM11] for the thin-plate spline in $\mathbb{R}^d$.

Points	Parameter		Error		Condition number	
	c_{L^∞}	c_{L^2}	L^∞	L^2	K_{L^∞}	K_{L^2}
n=16	30	6	$2.17 \cdot 10^{-4}$	$7.62 \cdot 10^{-5}$	$1.18 \cdot 10^{14}$	$1.75 \cdot 10^{8}$
n=32	50	55	$1.64 \cdot 10^{-4}$	$7.29 \cdot 10^{-5}$	$2.58 \cdot 10^{17}$	$2.58 \cdot 10^{17}$
n=64	35	1	$1.21 \cdot 10^{-4}$	$3.93 \cdot 10^{-5}$	$8.40 \cdot 10^{18}$	$4.48 \cdot 10^{15}$
n=128	3	3	$6.30 \cdot 10^{-9}$	$2.34 \cdot 10^{-9}$	$4.48 \cdot 10^{15}$	$2.50 \cdot 10^{15}$
n=256	1.5	1.5	$7.95 \cdot 10^{-12}$	$1.26 \cdot 10^{-12}$	$6.90 \cdot 10^{13}$	$3.53 \cdot 10^{13}$
n=512	1	1	$8.91 \cdot 10^{-13}$	$1.43 \cdot 10^{-13}$	$2.48 \cdot 10^{14}$	$1.24 \cdot 10^{14}$
n=1024	0.75	0.75	$9.60 \cdot 10^{-14}$	$1.81 \cdot 10^{-14}$	$8.11 \cdot 10^{17}$	$3.47 \cdot 10^{15}$
n=2048	0.45	0.45	$1.56 \cdot 10^{-13}$	$2.65 \cdot 10^{-14}$	$6.38 \cdot 10^{14}$	$6.38 \cdot 10^{14}$

Table 5.3: Error minimising values of c with the errors of the interpolation of f_1 and condition numbers of the corresponding interpolation matrices

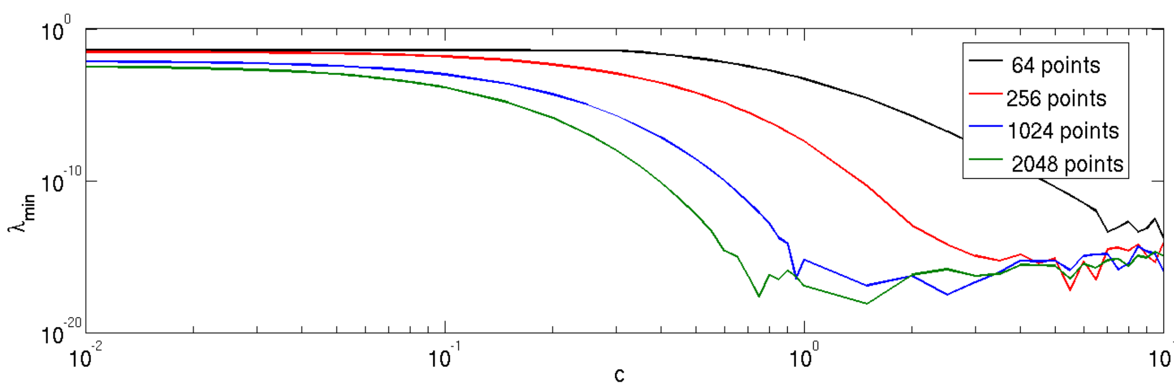

Figure 5.3: Minimal eigenvalue depending on c when using different point distributions

Points	Parameter			Error L^∞		
	c_{f_1}	c_{f_2}	c_{f_3}	f_1	f_2	f_3
n=16	9	2.5	1	$2.20 \cdot 10^{-4}$	$6.92 \cdot 10^{-4}$	$3.17 \cdot 10^{-1}$
n=32	4	4	0.8	$2.53 \cdot 10^{-4}$	$3.55 \cdot 10^{-5}$	$4.26 \cdot 10^{-3}$
n=64	2	2	1	$1.29 \cdot 10^{-4}$	$3.46 \cdot 10^{-7}$	$2.00 \cdot 10^{-4}$
n=128	1	1	1	$4.12 \cdot 10^{-7}$	$3.65 \cdot 10^{-7}$	$4.42 \cdot 10^{-5}$
n=256	0.9	0.9	0.9	$5.58 \cdot 10^{-9}$	$5.52 \cdot 10^{-9}$	$1.27 \cdot 10^{-7}$
n=512	0.55	0.55	0.55	$4.19 \cdot 10^{-9}$	$4.22 \cdot 10^{-9}$	$4.96 \cdot 10^{-9}$
n=1024	0.35	0.35	0.35	$2.79 \cdot 10^{-9}$	$2.81 \cdot 10^{-9}$	$3.20 \cdot 10^{-10}$
n=2048	0.2	0.2	0.2	$3.80 \cdot 10^{-9}$	$3.83 \cdot 10^{-9}$	$4.24 \cdot 10^{-9}$

Table 5.4: Error minimising values of c for φ_2 with the L^∞ errors of the interpolation of f_1, f_2 and f_3 when condition number is smaller than 10^{10}.

Since the problem of ill-conditioning arises for smaller values of c as the number of points increases, (see therefore the minimal eigenvalue of the interpolation matrix, as displayed in Figure 5.3) it would also be an option to apply partition of unity approaches for bigger numbers of data sites, the technique was for example described in [SL16] and also reduces the computational cost significantly.

Since we do not want to introduce new techniques at this point, we choose the optimal c under the condition that $K \leq 10^{10}$ is satisfied. Of course for different applications the upper margin should be chosen to meet the requirements of the application and our choice can only be considered an example. Since the different error measures did not lead to different optimal choices of c in the previous test we from now on focus on the L^∞ error estimate but want to investigate the influence of the test function and therefore compute the new values of c together with the error for all three test functions f_1, f_2 and f_3. The condition number for all the displayed choices of c and numbers of point is $\sim 10^9$. The results in Table 5.4 show that, by introducing a shift parameter, we can achieve a significant decrease of the error compared to the surface spline with $c = 0$ (Table 5.1) while keeping the condition number within a certain range. For an approximation of a good value of c, our results can be approximated by

$$c_{opt} \approx 30 \cdot 0.65^{\frac{\log(n)}{\log(2)}}$$

but the influence of the test function is bigger for a small number of points and our set of test functions is too small to allow for a general recommendation.

5.1.2 Comparison of the different basis functions

For the comparison of the basis functions we computed error estimates for interpolants to the described test functions of (5.1)-(5.3). We used the basis functions described in the beginning of this section and also give the condition number of the interpolation matrix.

We found that two categories have to be distinguished, the basis functions without an adjustable parameter and those with such a parameter. For the second group we chose approximately optimal parameters, as described for the shifted surface spline in Section 5.1.1, with the constrained of keeping the condition number of the interpolation matrix below 10^{10}. The detailed results for each of the functions are given in Appendix C.

The comparative results for the basis functions with an adjustable parameter are displayed in Table 5.5 for interpolation to a set of 64 points and in Table 5.6 and Table 5.7 for 256 and 1024 points. All methods lead to choosing a parameter that pushes the condition number to the given limit.

The results show that the optimal method depends on the number of points and the test function. All methods give good and mostly similar error results, the secans basis function performed better than the other methods for 1024 points but not as good as the other methods for 64 points.

We note the interesting fact that we do not find a specific basis function which works best for one test functions but it seems that different basis functions are more suitable for different point numbers (or separation distances). In our test we could identify the reciprocal multiquadric as performing best for 64 points. The Gaussian as best performing for 256 points and the shifted secans performing best for 1024 points.

We believe that this phenomenon is do to the upper limit we set to the condition number. The limit might induce the different basis functions to have an interval of the mesh distance in which they are able to achieve good results in terms of the error while keeping the condition number in the given range. But the tests we performed are not extensive enough to substantiate this conjecture.

For the functions without smoothing parameters we find that the surface spline performed best of the tested basis functions for all data distributions (Tables 5.8 to 5.10). The errors are larger than for the basis functions with smoothing but still good and the condition numbers are significantly smaller.

The compactly supported basis function did not perform as good as the other basis functions but we could find that a reduction of the support led to an decrease in the condition number while the error increased.

Method	Parameter			Error L^∞			K_∞		
	c_{f_1}	c_{f_2}	c_{f_3}	f_1	f_2	f_3	K_{f_1}	K_{f_2}	K_{f_3}
φ_2, STPS	2	2	1	0.000129	$3.46 \cdot 10^{-7}$	0.00020	$7.63 \cdot 10^8$	$7.63 \cdot 10^8$	$8.33 \cdot 10^9$
φ_3, GAU	1	0.3	2	0.000129	$\underline{2.54 \cdot 10^{-07}}$	0.000176	$3.60 \cdot 10^5$	$3.82 \cdot 10^9$	$3.40 \cdot 10^3$
φ_4, MQ	0.8	2.5	1	$\underline{0.000123}$	$3.03 \cdot 10^{-07}$	0.000435	$1.80 \cdot 10^5$	$8.14 \cdot 10^9$	$8.05 \cdot 10^5$
φ_5, IMQ	2	3.5	1.5	0.000128	$2.93 \cdot 10^{-07}$	$\underline{5.46 \cdot 10^{-05}}$	$6.70 \cdot 10^6$	$9.30 \cdot 10^9$	$2.926 \cdot 10^5$
φ_8, SEC	0.103	0.0856	0.00571	0.000386	0.000158	0.000985	9254	$1.11 \cdot 10^4$	$1.041 \cdot 10^5$

Table 5.5: Error minimising values of c with the L^∞ errors of the interpolation of f_1, f_2 and f_3 when condition number is smaller than 10^{10} for 64 points and different basis functions.

Basis function	Parameter	Error L^∞			K_∞
	c_{opt}	f_1	f_2	f_3	
φ_2, STPS	0.9	$5.58 \cdot 10^{-9}$	$5.52 \cdot 10^{-9}$	$1.27 \cdot 10^{-7}$	$9.22 \cdot 10^{9}$
φ_3, GAU	2.5	$\underline{3.89 \cdot 10^{-11}}$	$1.82 \cdot 10^{-09}$	$\underline{4.50 \cdot 10^{-08}}$	$5.89 \cdot 10^{9}$
φ_4, MQ	0.9	$1.32 \cdot 10^{-09}$	$\underline{4.66 \cdot 10^{-10}}$	$1.51 \cdot 10^{-07}$	$5.99 \cdot 10^{9}$
φ_5, IMQ	1	$6.44 \cdot 10^{-09}$	$1.83 \cdot 10^{-08}$	$1.71 \cdot 10^{-07}$	$8.92 \cdot 10^{7}$
φ_8, SEC	0.0571	$1.57 \cdot 10^{-8}$	$2.72 \cdot 10^{-08}$	$1.29 \cdot 10^{-07}$	$2.04 \cdot 10^{8}$

Table 5.6: Error minimising values of c with the L^∞ errors of the interpolation of f_1, f_2 and f_3 when condition number is smaller than 10^{10} for 256 points and different basis functions.

Basis function	Parameter	Error L^∞			K_∞
	c_{opt}	f_1	f_2	f_3	
φ_2, STPS	0.35	$2.79 \cdot 10^{-9}$	$2.81 \cdot 10^{-9}$	$3.20 \cdot 10^{-10}$	$8.53 \cdot 10^{9}$
φ_3, GAU	15	$8.79 \cdot 10^{-11}$	$2.32 \cdot 10^{-08}$	$2.1 \cdot 10^{-08}$	$1.01 \cdot 10^{9}$
φ_4, MQ	0.35	$1.49 \cdot 10^{-10}$	$\underline{2.35 \cdot 10^{-10}}$	$1.59 \cdot 10^{-09}$	$2.93 \cdot 10^{9}$
φ_5, IMQ	0.55	$2.48 \cdot 10^{-11}$	$1.08 \cdot 10^{-09}$	$2.5 \cdot 10^{-10}$	$2.44 \cdot 10^{9}$
φ_8, SEC	0.405	$\underline{1.32 \cdot 10^{-11}}$	$4.45 \cdot 10^{-10}$	$\underline{1.56 \cdot 10^{-10}}$	$7.53 \cdot 10^{9}$

Table 5.7: Error minimising values of c with the L^∞ errors of the interpolation of f_1, f_2 and f_3 when condition number is smaller than 10^{10} for 1024 points and different basis functions.

Basis function	Parameter	Error L^∞			K_∞
	c	f_1	f_2	f_3	
φ_1, TPS	$\star$	$1.62 \cdot 10^{-2}$	$1.62 \cdot 10^{-2}$	$3.24 \cdot 10^{-2}$	$3.73 \cdot 10^{3}$
φ_6, SRT	$\star$	$1.83 \cdot 10^{-2}$	0.0046	0.138	$4.33 \cdot 10^{3}$
φ_7, CSBF	π	$1.04 \cdot 10^{-2}$	$7.55 \cdot 10^{-2}$	$1.87 \cdot 10^{-1}$	$7.61 \cdot 10^{2}$
φ_7, CSBF	$\pi/2$	$3.5 \cdot 10^{-2}$	$2.55 \cdot 10^{-1}$	$6.32 \cdot 10^{-1}$	$3.86 \cdot 10^{1}$

Table 5.8: The L^∞ errors of the interpolation of f_1, f_2 and f_3 for 64 points and basis functions without smoothing parameter.

Basis function	Parameter	Error L^∞			K_∞
	c	f_1	f_2	f_3	
φ_1, TPS	$\star$	$9.65 \cdot 10^{-4}$	$9.87 \cdot 10^{-4}$	$2.73 \cdot 10^{-3}$	$2.13 \cdot 10^{4}$
φ_6, SRT	$\star$	$3.39 \cdot 10^{-3}$	$5.81 \cdot 10^{-4}$	$2.00 \cdot 10^{-2}$	$3.73 \cdot 10^{4}$
φ_7, CSBF	π	$2.40 \cdot 10^{-3}$	$1.65 \cdot 10^{-2}$	$4.07 \cdot 10^{-2}$	$2.42 \cdot 10^{4}$
φ_7, CSBF	$\pi/2$	$8.19 \cdot 10^{-3}$	$5.55 \cdot 10^{-2}$	$1.37 \cdot 10^{-1}$	$1.14 \cdot 10^{3}$

Table 5.9: The L^∞ errors of the interpolation of f_1, f_2 and f_3 for 256 points and basis functions without smoothing parameter.

Basis function	Parameter	Error L^∞			K_∞
	c	f_1	f_2	f_3	
φ_1, TPS	$\star$	$5.87 \cdot 10^{-5}$	$6.21 \cdot 10^{-5}$	$1.59 \cdot 10^{-4}$	$3.41 \cdot 10^{5}$
φ_6, SRT	$\star$	$4.28 \cdot 10^{-4}$	$6.83 \cdot 10^{-5}$	$4.58 \cdot 10^{-3}$	$2.85 \cdot 10^{5}$
φ_7, CSBF	π	$4.20 \cdot 10^{-4}$	$2.84 \cdot 10^{-3}$	$7.03 \cdot 10^{-3}$	$7.76 \cdot 10^{5}$
φ_7, CSBF	$\pi/2$	$1.44 \cdot 10^{-3}$	$9.73 \cdot 10^{-3}$	$2.41 \cdot 10^{-2}$	$3.61 \cdot 10^{4}$

Table 5.10: The L^∞ errors of the interpolation of f_1, f_2 and f_3 for 1024 points and basis functions without smoothing parameter.

In the next section we will test the described techniques on a real life application, to see if we find similar results.

5.2 Using spherical basis functions for reconstruction of electroencephalographic data

An electroencephalogram (EEG) evaluates electrical activity produced by the brain, most commonly it is used to detect seizure disorders but it also frequently used for research on the functioning of the brain. In electroencephalography the electrical activity in the brain is recorded by electrodes placed on the surface of the scalp. The resulting traces are known as an EEG and are used by researchers to determine the level of activity in certain areas of the brain.

The reconstruction of data by interpolation methods is of great practical interest in the research on electroencephalography as it is a basis for brain-mapping of multichannel data. In addition, interpolation algorithms can be used for the reconstruction of missing data, which were lost due to technical problems. Such as broken electrodes or by technical or physiological artefacts (e.g., loosening of the electrode or blinking of the participant). Methods stemming from approximation theory have been applied to this problem, yet several difficulties remain to this date. There are problems computing the reconstruction, and with most methods used, there is an error increase when the corner electrodes are to be reconstructed. In this section we investigate whether the application of radial basis functions has advantages as compared to the commonly used nearest-neighbour averaging. In addition, we are interested in whether the radial basis approximants are easier and faster to compute. Since, a spherical model is the simplest resembling the real anatomical setting, we applied the spherical basis functions tested in the last section to the problem of reconstruction of EEG data.

First tests for this application were included in [Jäg14], where the data was recorded using a 64 electrode EEG mask and there were only 6 sets of test data. Now we use a broader set of spherical basis functions and data recorded using a 32 multichannel EEG. The recordings stem from 10 healthy volunteers recorded in four different recording situations. Parts of the results of this section have already been published in [JKBS16], but we now add the shifted surface spline, the secans and the Gaussian basis function to the test.

To have a benchmark of existing methods we used a commonly used nearest neighbour technique and compared the methods using a leave one out and leave two out cross-validation.

The nearest-neighbour technique (NN) has been widely used for reconstruction and interpolation of EEG data, for our test we used an implementation by Alexander Klein.

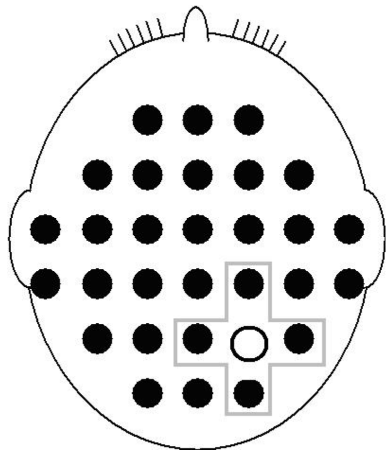

Figure 5.4: Distribution of the electrodes on the head, as seen from above, with an example of the nearest neighbours of an electrode.

The estimated value at a point p by the k^{th} nearest-neighbour method is given by:

$$v(p) = \text{mean}\left(\{v(p_1), \ldots, v(p_k)\}\right),$$

where $p_1, \ldots, p_k$ denote the positions of the k nearest neighbour electrodes and $v(p_i)$ is the potential measured at this point. The neighbours were determined from the arrangement shown in Figure 5.4. In our study we use a maximum of $k = 4$ neighbouring electrodes. We did not weight the electrodes by their distance from the electrode to be reconstructed, because they are nearly uniformly distributed. The 30 electrodes were regularly spaced starting at the inion (point at the back of the skull), and extended in steps of 15 % of the nasion-inion distance (distance between the back of the skull and the point between the eyes) to 5 % anterior of F_z (the electrode on the forehead). The minimal number of neighbours possible in this set-up is 2.

The radial basis function method requires using the electrode positions in the 3-dimensional Euclidean space. We denote $p_i = (x_i, y_i, z_i)$ as the position of the i-th electrode. We chose the 2-sphere of radius one as a model for the scalp, the electrode positions are therefore given as distributed on $\mathbb{S}^2$. This choice has the advantage that the information accompanying the EEG-mask used, often include these kind of coordinate-distribution.

We compared the nearest-neighbour technique (NN) to the spherical basis function interpolants with the basis functions

$$\begin{aligned}
\varphi_2(x) &= (2-2x+c^2)\log(2-2x+c^2),\ \ c>0, \text{ shifted surface spline,}\\
\varphi_3(x) &= e^{-\alpha(2-2x)},\ \ \alpha>0, \text{ Gaussian ,}\\
\varphi_4(x) &= \sqrt{c^2+2-2x}, \text{ multiquadric,}\\
\varphi_5(x) &= \frac{1}{2-2x+c^2},\ \ c>0, \text{ spherical reciprocal multiquadric,}\\
\varphi_8(x) &= \frac{1}{\cos(x+c)},\ \ c>0, \text{ shifted secans,}
\end{aligned}$$

which have given good results in the test described in the previous section.

5.2.1 Methods used for the evaluation of the interpolation

The data investigated was derived from 30-channel full-scalp EEG measurements of 10 normal subjects, randomly chosen from data recorded in the course of the doctoral dissertation [Wü13]. The EEG was amplified with a Braintronics ISO 1032 amplifier and digitised at a rate of 500 Hz, with the time-constant for the input set to 0.3 s (equivalent to highpass-filtering with a cut-off frequency of 0.53 Hz), a notch filter rejecting mains hum at 50 Hz, and a high cut-off of 70 Hz at 24 db per octave. All of the subjects were recorded in 4 situations. The data was recorded by Martin Würzer and the preprocessing using the described filters and the selection of the artefact free samples were performed by Alexander Klein. This way 40 samples free of technical artefacts of length 5 s where chosen (2501 points in time), hence every of the 40 measurements included 72529 data points. We evaluated the methods by using a leave one out cross-validation. The value at each site was predicted using the information of the remaining electrode sites and compared to the actual value. The error was determined as

$$MSE = \frac{1}{n_e \cdot n_e} \left\| Y - \widetilde{Y} \right\|_{Frob}^2$$

where $\widetilde{Y}$ denotes the matrix of the measured data, with the measurements each electrode to be reproduced in one row and each time of measurement in one column, and Y denotes the predicted data in the same form and n_e is the number of electrodes to be reconstructed and n_t is the number of points in time.

5.2.2 Results

We choose the smoothing parameters to minimise the mean square error of the interpolation over all sets investigated and all parameters tested, by leave one out cross-validation. We used the same parameters for the leave two out cross-validation, because the distribution of the data sites is only slightly changed by leaving out another electrode. In distinction to the results in the previous section, where we computed interpolants to smooth test functions, we were able to find an error minimising value of the smoothing parameter for each basis function which is not minimum due to the growing condition number of the interpolation matrix. We also note that this optimal parameter yields less smooth basis functions then were approximately optimal for 32 points of the smooth test functions in the previous section.

The basis functions with their optimal parameters are

$$\begin{aligned}
\varphi_2(x) &= (2-2x+c^2)\log(2-2x+c^2),\ c=0.001, \text{ shifted surface spline},\\
\varphi_3(x) &= e^{-\alpha(2-2x)},\ \alpha = 3.65, \text{ Gaussian},\\
\varphi_4(x) &= \sqrt{c^2+2-2x},\ c=0.05, \text{ multiquadric},\\
\varphi_5(x) &= \frac{1}{2-2x+c^2},\ c=0.55, \text{ spherical reciprocal multiquadric},\\
\varphi_8(x) &= \frac{1}{\cos(x+c)},\ c=0.35, \text{ shifted secans.}
\end{aligned}$$

Each technique was used to determine the error in predicting the potential at one or two electrode sites from the potentials recorded at the others. The mean square error and maximal error of the cross-validation for leave one out and leave two out tests are given in Table 5.11.

In this comparison we manly focus on the mean square error because even though the samples were chosen not to include any visible artefact there can still be non detected artefact in the data which influence the maximal error.

Our results show that the global techniques perform better than the local technique. This matches the results of [STRL$^+$91], where the performance of interpolation techniques was compared. The techniques included thin-plate splines and spherical splines, but not the multiquadric, Gaussian or secans methods. Comparing the multiquadric methods to the nearest-neighbour technique we see a significant decrease of the error. We have to mention here that for the leave two out cross validation, when a corner electrode and its neighbouring electrode are reconstructed, the data of the corner electrode will simply be overwritten with the data of the only remaining neighbour. This means

Method /Parameter	Leave one out		Leave two out	
	mean square error	max error	mean square error	max error
NN	10.9597 μV^2	48.778 μV	11.3199 μV^2	62.0257 μV
TPS / $c = 0$	9.2218 μV^2	48.1267 μV	9.3726 μV^2	48.8293 μV
GAU / $c = 3.65$	11.0589 μV^2	37.9109 μV	11.2911 μV^2	44.9521 μV
MQ / $c = 0.05$	8.2760 μV^2	44.2835 μV	8.4069 μV^2	40.7785 μV
IMQ / $c = 0.55$	8.7775 μV^2	40.7270 μV	8.9388 μV^2	40.7785 μV
SEC / $c = 0.35$	9.1922 μV^2	42.193 μV	9.3079 μV^2	42.2670 μV

Table 5.11: Error of the leave one out and leave two out cross-validation of the EEG

the nearest neighbour technique is not really applicable for the reconstruction of two or more electrodes. We also find that in this small study the multiquadric and reciprocal multiquadric techniques give the best results. The results are slightly better than those of the thin-plate spline and the secans and significantly better than the results achieved using Gaussian interpolation. This is an important result since the Gaussian basis function is widely used.

We conclude that the best results were achieved using multiquadric interpolation. For all these reasons, we decided on the multiquadric interpolation as best suited for reconstructing EEG data. It showed good results and can be calculated easily. This is why we implemented this technique for data reconstruction and the physiology department of the Justus-Liebig university is currently using it.

Chapter 6

Summary and future work

We now briefly summarize the most important results of this thesis:

- We have studied the class of multiply monotone functions and generalised results previously known for completely monotone functions to this class as well as introduced new results.

- We employed these results to construct new radial basis functions, which are for example exponential splines.

- We studied shifts of radial basis functions on $\mathbb{R}^d$ and $\mathbb{S}^{d-1}$ and gave a formula for the computation of their Fourier transform in the first case.

- We computed a series representation for the inverse Gaussian class of radial basis functions.

- We gave several new sufficient results for the (conditionally) positive definiteness of spherical functions, which make use of their monotonicity properties.

- We computed the Gegenbauer coefficients of the shifted surface spline and proved that they decay exponentially, which is important to derive error estimates of their interpolation.

- We tested and compared new and well known spherical basis functions on smooth test functions and using data recorded from an EEG.

We can summarise that the described new results for multiply monotone functions together with the results on positive definiteness in Section 4.2 allow us to construct new basis functions for interpolation. We still have to admit that using only multiply monotone functions has the draw back, that those functions will always be non differentiable in zero. We find that this problem can be easily addressed by applying the dimension hopping techniques of Wendland for Euclidean basis functions and of Beatson and zu Castell for the sphere. We included their results in Appendix A. The described results allow the construction of smoother basis functions via dimension walk. The smoothness of the basis function is increased while the dimension of the positive definiteness is reduced. The well known Wendland functions are a result of this technique, when the function to which the operators are applied is the truncated power, but the operators described in the Appendix can also be applied to any multiply monotone functions described in Chapter 2, so that we are also able to produce new smooth basis functions.

For spherical basis functions we note that our results demonstrate how important monotonicity properties are also for those functions. Most of our results apply to functions which are positive definite on spheres of arbitrary dimension. The monotonicity properties and smoothness conditions of functions which are only positive definite up to certain dimension remain a subject further research is required on.

We further introduced a possible way of scaling spherical basis functions but the problem described by Gneiting, to be precise: The question for which types of functions and which values of $c \in \mathbb{R}$ the implication

$$\phi \in SPD(\mathbb{S}^{d-1}) \quad \to \quad \phi\left(\frac{\cdot}{c}\right) \in SPD(\mathbb{S}^{d-1})$$

holds is still an open problem. We hope to solve it using the insight derived from the work on this thesis.

We will also try to add the missing part of Problem 2 proposed by Gneiting which reads:

$$\text{Does } \phi \in SPD(\mathbb{R}^{d-1}) \text{ with } \phi(t) = 0 \text{ for all } t \geq \pi \text{ imply } \phi \in SPD(\mathbb{S}^{d-1})?$$

We hope to be able to prove the conjecture using a generalisation of the work of Xu [Xu18]. The results we already achieved together with the conjectures which we still need to prove are described in Appendix C.

Appendix A

Techniques to construct smooth basis functions

In this appendix we describe ways of consrtucting basis functions for the sphere and on $\mathbb{R}^d$. We will present two closely connected techniques, the first of those was originally introduced by Wendland in [Wen96]. These techniques are of special interest to us because they can be applied to the new functions which we introduced in the previous chapters, furthermore they can be used to derive smoother basis functions from multiply monotone functions.

A.1 Constructing Euclidean basis functions via dimension walk

The Euclidean version of the dimension walk makes use of a property of the derivatives of Bessel functions. A full description of the techniques including the proofs is given in [SW01]. For the Bessel functions the following is true

$$\frac{d}{dz}\left\{z^\nu J_\nu(z)\right\} = z^\nu J_{\nu-1}(z).$$

This property can be used to give a new characterisation of the d-dimensional Fourier transform

$$F_d\phi(r) = F_{d-2}\left(\int_\bullet^\infty \phi(s)s\,ds\right)(r)$$

if the boundary terms of the integral vanish. By defining the operators

$$I\phi(r) := \int_r^\infty \phi(t)t\,dt \tag{A.1}$$

and

$$D\phi(r) := \frac{-1}{r}\frac{d}{dr}\phi(r) \tag{A.2}$$

an alternative construction method of strictly positive definite functions is derived.

Theorem A.1. *If $\phi \in [0,\infty)$ satisfies $t \to \phi(t)t^{d-1} \in L^1[0,\infty)$ for some $d \geq 3$, then we have that*

$$F_d(\phi) = F_{d-2}(I\phi).$$

This means ϕ is strictly positive definite on $\mathbb{R}^d$ if and only if $I\phi$ is strictly positive definite on $\mathbb{R}^{d-2}$. On the other hand if for some $d \geq 1$, ϕ satisfies $t \to \phi(t)t^{d-1} \in L^1[0,\infty)$ and $\phi(t) \to 0$ at $t \to \infty$ and if the even extension of ϕ to $\mathbb{R}$ is in $C^2(\mathbb{R})$ then

$$F_d(\phi) = F_{d+2}(D\phi).$$

So that ϕ is strictly positive definite on $\mathbb{R}^d$ if and only if $D\phi$ is strictly positive definite on $\mathbb{R}^{d+2}$.

Wendland constructed, using this theorem, the class of so called Wendland functions which are derived from the truncated power function.

Theorem A.2. *Define $\phi_\ell(r) = (1-r)_+^\ell$ and $\phi_{d,k}$ by*

$$\phi_{d,k} = I^k \phi_{\lfloor d/2 \rfloor + k + 1}. \tag{A.3}$$

Then $\phi_{d,k}$ is compactly supported, a polynomial within its support, and positive definite on $\mathbb{R}^d$.

A.2 Constructing spherical basis functions via dimension walk

Interesting new techniques for the construction of spherical basis functions were recently described by Beatson and zu Castell [BzC17]. They allow a construction of compactly supported functions on the sphere analogue to the one described by Wendland for Euclidean spaces. The described montée and descent operators can also be combined with new basis functions which can be constructed from Section 4.2.

Definition A.3. *Given f absolutely continuous on $[-1,1]$ define Df by*

$$Df(x) = f'(x), \quad x \in [-1,1]. \tag{A.4}$$

Also, given f integrable on $[-1,1]$ define an operator I by

$$If(x) = \int_{-1}^{x} f(u)\, du. \tag{A.5}$$

The operators are under some mild conditions preserving strict positive definiteness on spheres. The reasons for this is their action on the Gegenbauer polynomials

$$DC_n^\lambda = \begin{cases} 2\lambda C_{n-1}^{\lambda+1}, & \lambda > 0, \\ 2C_{n-1}^{1}, & \lambda = 0. \end{cases}$$

We define

$$\mu_\lambda = \begin{cases} \lambda, & \lambda > 0. \\ 1, & \lambda = 0, \end{cases}$$

then

$$IC_{n-1}^{\lambda+1} = \frac{1}{2\mu_\lambda}\left(C_n^\lambda - C_n^\lambda(-1)\right), \quad \lambda \geq 0.$$

We sum up the results on the operators, as is clear from the above the operators are defined for spherical basis functions given in the form $\varphi : [-1,1] \to \mathbb{R}$.

Theorem A.4.
- *Let $d \geq 1$ and $\varphi(\cos(\cdot)) \in SPD(\mathbb{S}^{d+1})$ then there is a constant C such that $(C + I\varphi)(\cos(\cdot)) \in SPD(\mathbb{S}^{d-1})$.*
- *Let $d \geq 2$ and $\varphi(\cos(\cdot)) \in SPD(\mathbb{S}^{d-1})$ have a derivative $\varphi' \in C[-1,1]$, then $(D\varphi)(\cos(\cdot)) \in SPD(\mathbb{S}^{d+1})$.*

The montée operator can be used to construct smoother basis functions from less smooth functions which are positive definite in higher dimensions.

Example A.5. *Choosing the cut of potential*

$$f_m(\cos(\theta)) = (t-\theta)_+^m, \quad 0 < \theta < \pi.$$

We can derive the following functions which are strictly positive definite on $\mathbb{S}^3$,

$$I f_3(\cos(\theta)) = \\ = \begin{cases} \cos(\theta)\left((t-\theta)^3 - 6(t-\theta)\right) + \sin(\theta)\left(3(t-\theta)^2 - 6\right) + 6\sin(t), & 0 \leq \theta < t, \\ 0, & t \leq \theta \leq \pi, \end{cases} \tag{A.6}$$

and

$$\begin{aligned}(I^2 f_4)(\cos(\theta)) = {}& \cos(2\theta)\left(\frac{1}{4}(t-\theta)^4 - \frac{21}{4}(t-\theta)^2 + \frac{93}{8}\right) \\ & + \sin(2\theta)\left(\frac{3}{2}(t-\theta)^3 - \frac{45}{4}(t-\theta)\right) \\ & - 24\cos(\theta)\cos(t) + \left(\frac{1}{2}(t-\theta)^4 - 6(t-\theta)^2 + \frac{3}{4}\cos^2(t) + \frac{93}{8}\right),\end{aligned}$$

for $0 \leq \theta < t$, *and* $(I^2 f_4)$ *is equal to zero for* $t \leq \theta \leq \pi$.

Appendix B

Generating point sets for numerical tests on the sphere

There are many different approaches to generate sets of points to test spherical approximation methods. We will describe here the one we used in our test. The technique tries to mimic a grid on the sphere in a way that the distance between neighbouring points in two orthogonal directions is similar. This techniques was described in [Des04].

We will create a set of approximately n points. The idea is to divide the area of the sphere into n squares. The length of one side of such a square would then be $d = \sqrt{4\pi/n}$. We then produce $M_\theta = \lfloor \pi/d \rfloor$ circles on the sphere and produce on each circle a number of points proportional to the length of this circle. Two examples, one of approx. 100 and one of approximately 1000 points, distributed using the described method are displayed in Figure B.1. To use the sets for numerical evaluation we need to estimate the number

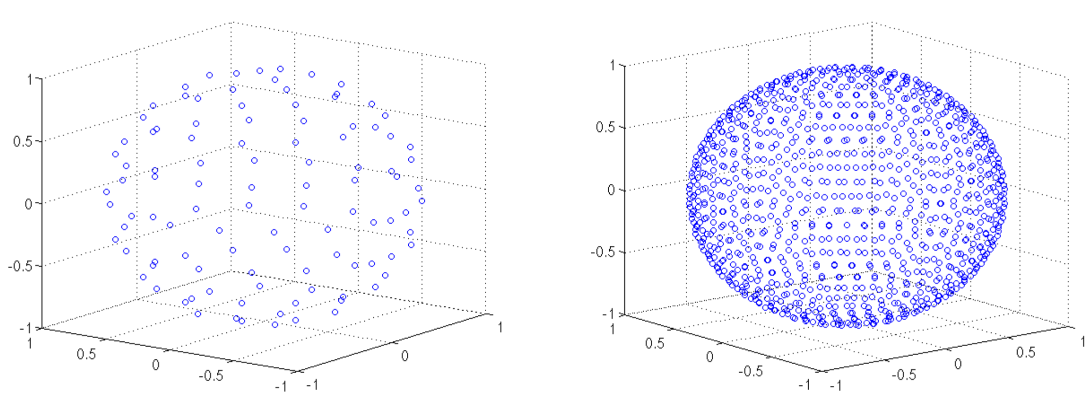

Figure B.1: Regular distributed data points for $n = 100$ and for $n = 1000$

n	n_r	h_r	$\sqrt{\frac{2\pi}{n}}$
16	20	0.5874	0.6267
32	32	0.4403	0.4431
64	64	0.3207	0.3133
128	128	0.2262	0.2216
256	250	0.1674	0.1567
512	508	0.1104	0.1108
1024	998	$0.78872 \cdot 10^{-1}$	$0.7833 \cdot 10^{-1}$
2048	2038	$0.5522 \cdot 10^{-1}$	$0.5539 \cdot 10^{-1}$
4096	4136	$0.3782 \cdot 10^{-1}$	$0.3917 \cdot 10^{-1}$

Table B.1: Real number of points and mesh norm of the described sphere set compared to their approximation

of points and the mesh distance of the resulting sets. To do so we will compare the actual number of points $n_r = |\Xi|$ with the number of points used for the construction n and an approximation of the resulting mesh distance of the set Ξ, $h_r = \sup_{\zeta \in \mathbb{S}^{d-1}} \min\{\cos^{-1}(\zeta^T \xi) : \xi \in \Xi\}$ with our approximation $h = \sqrt{\frac{2 \cdot \pi}{n}}$. The results were computed using the Octave software, here the mesh norm h_r is approximated as the maximum of a discrete set of 10000 points. We display the results in table B.1. We see that the the value n is a good estimate for the number of points and the value h is a good estimate for the mesh distance of the point set.

Appendix C

Additional numerical results

In this appendix we give numerical results for the interpolation on the sphere using different spherical basis functions. The results are used in the comparison given in Section 5.1. The functions considered are:

$$\varphi_3(x) = e^{-\alpha(2-2x)}, \; \alpha > 0, \text{ Gaussian,} \tag{GAU}$$
$$\varphi_4(x) = \sqrt{c^2+2-2x}, \text{ multiquadric,} \tag{MQ}$$
$$\varphi_5(x) = \frac{1}{2-2x+c^2}, \; c > 0, \text{ spherical reciprocal multiquadric,} \tag{IMQ}$$
$$\varphi_6(x) = -\frac{1}{\pi}\left(\frac{\pi}{2} + \arccos(x)\right)^{1/2}, \text{ new s.b.f. from Example 4.31,} \tag{SRT}$$
$$\varphi_7(x) = If_4(x) = \int_{-1}^{x} (t - \arccos(\theta))_+^4 \, d\theta, \text{ compactly supported s.b.f. from [BzC17],} \tag{CSBF}$$
$$\varphi_8(x) = \frac{1}{\cos(x+c)}, \; c > 0, \text{ shifted secans.} \tag{SEC}$$

The first three basis functions have already been used in tests and applications, the other ones were introduced in this thesis and we study their numerical stability and accuracy properties more thoroughly.

The test functions used to derive error estimates are, as in Chapter 5:

$$f_1(\xi) = \sin(\xi_1)\sin(\xi_2)\sin(\xi_3),$$
$$f_2(\xi) = \frac{25}{25 + (\xi_1 - 0.2)^2 + 2\xi_2 + \xi_3},$$
$$f_3(\xi) = e^{\xi_1^2}.$$

To be able to compare the performance of the basis functions we apply the basis functions to the same tests which were used in Section 5.1 to study the surface spline and the shifted surface spline. For the functions which have not been considered before we add some exploratory tests to study their stability and accuracy.

C.1 Results on the Gaussian basis function for the sphere

The behaviour of the Gaussian basis function (dependent on the smoothing parameter) is well studied in the Euclidean setting (for example in [DF02] and [FWL04]). The Gaussian becomes increasingly flat for $\alpha \to 0$. The error when approximating smooth functions usually decays in this case until the interpolation matrix becomes too ill condition for computation. For Euclidean basis functions there have been techniques developed to overcome this problem but for the sphere we for now accept the resulting restrictions and choose a smoothing parameter which results in an interpolation matrix with $K_\infty \leq 10^{10}$.

We proceed similarly to the investigation of the shifted thin-plate spline (in Section 5.1) and choose for each of the three test functions the error minimising value of α for different point numbers. The construction of our test set is described in Appendix B, for this point set on the sphere. Since we consider smooth test functions and do not include noise in our tests the L^∞ error is a good tool to evaluate the performance of the method. We want to study the influence of the test function and therefore compute approximately optimal values of α together with the error for all three test functions f_1, f_2 and f_3. The results are displayed in Table C.1. The condition number for all the displayed choices of α and numbers of point is $\sim 10^9$.

C.2 Results on the multiquadric and reciprocal multiquadric basis functions for the sphere

The behavior of the multiquadric basis function in relation to the smoothing parameter was for example studied in [Rip99]. The multiquadric becomes increasingly flat for $c \to \infty$. The error in this case usually decays until the interpolation matrix becomes too ill conditioned for computation. Since the condition number increases for $c \to \infty$ we will choose a smoothing parameter which results in an interpolation matrix with $K_\infty \leq 10^{10}$.

We proceed similarly to the investigation of the shifted surface spline and the Gaus-

Points	Best parameter			Error L^∞		
	α_{f_1}	α_{f_2}	α_{f_3}	f_1	f_2	f_3
$n = 16$	0.0095	0.35	0.65	0.000217	0.000705	0.32
$n = 32$	0.07	0.55	1.5	0.000245	$2.75 \cdot 10^{-05}$	0.00393
$n = 64$	1	0.3	2	0.000129	$2.54 \cdot 10^{-07}$	0.000176
$n = 128$	0.95	0.95	0.95	$6.79 \cdot 10^{-09}$	$1.33 \cdot 10^{-09}$	$2.8 \cdot 10^{-05}$
$n = 256$	2.5	2.5	2.5	$3.89 \cdot 10^{-11}$	$1.82 \cdot 10^{-09}$	$4.50 \cdot 10^{-08}$
$n = 512$	6	6	6	$2.00 \cdot 10^{-11}$	$2.40 \cdot 10^{-09}$	$2.03 \cdot 10^{-09}$
$n = 1024$	15	15	15	$8.79 \cdot 10^{-11}$	$2.32 \cdot 10^{-08}$	$2.10 \cdot 10^{-08}$

Table C.1: Error minimising values of α for the Gaussian φ_3 with the L^∞ errors of the interpolation of f_1, f_2 and f_3 when condition number is smaller than 10^{10}.

Points	Best parameter			Error L^∞		
	c_{f_1}	c_{f_2}	c_{f_3}	f_1	f_2	f_3
$n = 16$	10	2	1.5	0.000221	0.000717	0.318
$n = 32$	4.5	1.5	0.9	0.000252	$3.13 \cdot 10^{-05}$	0.00176
$n = 64$	0.8	2.5	1	0.000123	$3.03 \cdot 10^{-07}$	0.000435
$n = 128$	1	1	1	$3.83 \cdot 10^{-07}$	$3.25 \cdot 10^{-08}$	$4.91 \cdot 10^{-05}$
$n = 256$	0.9	0.9	0.9	$1.32 \cdot 10^{-09}$	$4.66 \cdot 10^{-10}$	$1.51 \cdot 10^{-07}$
$n = 512$	0.55	0.55	0.55	$7.64 \cdot 10^{-10}$	$1.76 \cdot 10^{-10}$	$1.45 \cdot 10^{-09}$
$n = 1024$	0.35	0.35	0.35	$1.49 \cdot 10^{-10}$	$2.35 \cdot 10^{-10}$	$1.59 \cdot 10^{-09}$

Table C.2: Error minimising values of c for the multiquadric φ_4 with the L^∞ errors of the interpolation of f_1, f_2 and f_3 when condition number is smaller than 10^{10}.

sian, by choosing for each of the three test functions the error minimising value of c for different point numbers from the set of tested values of c. We display the results in Table C.2. The condition number for all the displayed choices of c and numbers of point is $\sim 10^9$.

For the reciprocal multiquadric (IMQ) we compute about optimal choices of the value c. The reciprocal multiquadrics becomes increasingly flat for $c \to \infty$. The error decays in this case until the interpolation matrix becomes too ill conditioned for computation. We again choose a smoothing parameter which results in an interpolation matrix with $K_\infty \leq 10^{10}$.

The test method is the same as described for the previous functions. The results are displayed in Table C.3. The condition numbers for all the displayed choices of α and numbers of point are again $\sim 10^9$.

Points	Best parameter			Error L^∞		
	c_{f_1}	c_{f_2}	c_{f_3}	f_1	f_2	f_3
$n = 16$	15	3	2	0.000219	0.000723	0.319
$n = 32$	6.5	2.5	1.5	0.000248	$3 \cdot 10^{-05}$	0.00492
$n = 64$	2	3.5	1.5	0.000128	$2.93 \cdot 10^{-07}$	$5.46 \cdot 10^{-05}$
$n = 128$	2	2	2	$1.59 \cdot 10^{-08}$	$1.27 \cdot 10^{-09}$	$2.98 \cdot 10^{-05}$
$n = 256$	1	1	1	$6.44 \cdot 10^{-09}$	$1.83 \cdot 10^{-08}$	$1.71 \cdot 10^{-07}$
$n = 512$	0.85	0.85	0.85	$7.24 \cdot 10^{-11}$	$3.91 \cdot 10^{-10}$	$2.18 \cdot 10^{-10}$
$n = 1024$	0.55	0.55	0.55	$2.48 \cdot 10^{-11}$	$1.08 \cdot 10^{-09}$	$2.500 \cdot 10^{-10}$

Table C.3: Error minimising values of c for the reciprocal multiquadric φ_5 with the L^∞ errors of the interpolation of f_1, f_2 and f_3 when condition number is smaller than 10^{10}.

Points	Error L^∞	Error L^2	k_∞	k_2	K_{L^∞}
$n = 16$	0.0801	0.0304	$\star$	$\star$	460
$n = 32$	0.0444	0.0261	1.7	0.439	$1.67 \cdot 10^{+03}$
$n = 64$	0.0183	0.00684	2.56	3.86	$4.33 \cdot 10^{+03}$
$n = 128$	0.00947	0.00383	1.9	1.68	$1.37 \cdot 10^{+04}$
$n = 256$	0.00339	0.00139	2.96	2.92	$3.73 \cdot 10^{+04}$
$n = 512$	0.00122	0.000434	2.96	3.36	$1.07 \cdot 10^{+05}$
$n = 1024$	0.000428	0.000155	3.02	2.97	$2.85 \cdot 10^{+05}$
$n = 2048$	0.000126	$4.67 \cdot 10^{-05}$	3.52	3.46	$8.68 \cdot 10^{+05}$

Table C.4: Estimate of the convergence order of the shifted root φ_6 for testfunction f_1

C.3 Results on the shifted root basis function for the sphere

The shifted root basis function was given as an example of a basis function constructed in Section 4, Example 4.31. The basis function was not considered before and we start to study it without an additional smoothing parameter. We show in Table C.4 the L^2 and L^∞-error of the interpolation to test function f_1 together with the estimated convergence rate. The computation was repeated with the test functions f_2 (see Table C.5) and f_3 (see Table C.6). Even though we have not computed the decay rate of the Fourier coefficients of this basis functions the results suggest that the convergence rate of the error might be near 2.

Points	Error L^∞	Error L^2	k_∞	k_2	K_{L^∞}
$n = 16$	0.0238	0.00811	$\star$	$\star$	460
$n = 32$	0.00908	0.0029	2.78	2.96	$1.67 \cdot 10^{+03}$
$n = 64$	0.00448	0.00152	2.04	1.87	$4.33 \cdot 10^{+03}$
$n = 128$	0.00145	0.000411	3.25	3.77	$1.37 \cdot 10^{+04}$
$n = 256$	0.000581	0.000156	2.65	2.78	$3.73 \cdot 10^{+04}$
$n = 512$	0.000217	$6.48 \cdot 10^{-05}$	2.84	2.54	$1.07 \cdot 10^{+05}$
$n = 1024$	$6.83 \cdot 10^{-05}$	$2.05 \cdot 10^{-05}$	3.34	3.33	$2.85 \cdot 10^{+05}$
$n = 2048$	$3.04 \cdot 10^{-05}$	$7.93 \cdot 10^{-06}$	2.33	2.73	$8.68 \cdot 10^{+05}$

Table C.5: Estimate of the convergence order of the shifted root φ_6 for testfunction f_2

Points	Error L^∞	Error L^2	k_∞	k_2	K_{L^∞}
$n = 16$	0.933	0.251	$\star$	$\star$	460
$n = 32$	0.194	0.0791	4.54	3.33	$1.67 \cdot 10^{+03}$
$n = 64$	0.138	0.043	0.978	1.76	$4.33 \cdot 10^{+03}$
$n = 128$	0.0509	0.0118	2.88	3.74	$1.37 \cdot 10^{+04}$
$n = 256$	0.02	0.00446	2.69	2.8	$3.73 \cdot 10^{+04}$
$n = 512$	0.0133	0.00237	1.19	1.82	$1.07 \cdot 10^{+05}$
$n = 1024$	0.00458	0.000752	3.07	3.31	$2.85 \cdot 10^{+05}$
$n = 2048$	0.00177	0.000303	2.74	2.62	$8.68 \cdot 10^{+05}$

Table C.6: Estimate of the convergence order of the shifted root φ_6 for testfunction f_3

Points	Best parameter			Error L^∞		
	t_{f_1}	t_{f_2}	t_{f_3}	f_1	f_2	f_3
$n = 16$	3.14	3.14	3.14	0.0382	0.0208	0.387
$n = 32$	3.14	3.14	3.14	0.00744	0.00631	0.0241
$n = 64$	3.14	3.14	3.14	0.00146	0.00111	0.00901
$n = 128$	3.14	3.14	2.34	0.000219	0.000185	0.00188
$n = 256$	3.14	3.14	2.49	$3.41 \cdot 10^{-05}$	$3.46 \cdot 10^{-05}$	0.000298
$n = 512$	3.14	3.14	2.59	$5.56 \cdot 10^{-06}$	$5.49 \cdot 10^{-06}$	$5.11 \cdot 10^{-05}$
$n = 1024$	3.14	3.14	2.69	$1.1 \cdot 10^{-06}$	$1.01 \cdot 10^{-06}$	$8.06 \cdot 10^{-06}$

Table C.7: Error minimising values of c for the compactly supported sbf φ_7 with the L^∞ errors of the interpolation of f_1, f_2 and f_3 when condition number is smaller than 10^{10}.

C.4 Results on the compactly supported spherical basis function of Beatson and zu Castell

We compute close to optimal choices of the value $0 < t < \pi$ for the compactly supported basis function introduced in [BzC17]. These functions have to our knowledge not been examined in numerical tests, so we start computing errors and conditions numbers for 100 values of t equally distributed in the interval $(0, \pi)$.

To compare the performance to the other basis functions we choose again an approximately optimal parameter t which minimises the maximal error while keeping the condition number smaller then 10^{10}. The results are shown in Table C.7. We find that the methods achieves the best results when we choose a maximal support of the basis function, which is equivalent to setting $t = \pi$. We also give the L^∞ and L^2 error estimates together with the condition number and estimates of the convergence order, for $t = \pi$ in Table C.8 and for $t = \pi/2$ in Table C.9. We find that reducing the size of the support decreases the condition number and increases the error as we expected. We did not find a difference in the estimates of the convergence order. We believe that the benefits of the compact support would only be significant for a number of points $\gg 1000$.

C.5 Results on the shifted secans

We compute approximately optimal choices of the value $0 < \tau < \frac{\pi}{2} - 1$ for the shifted secans. These functions have to our knowledge not been considered before so we started computing errors and conditions numbers for 100 values of τ equally distributed in the interval $\left(0, \frac{\pi}{2} - 1\right)$. The connection of condition and the shift parameter τ is displayed in

Points	Error L^∞	Error L^2	k_∞	k_2	K_{L^∞}
$n = 16$	0.0302	0.0114	10.1	12.9	35.9
$n = 32$	0.0226	0.00803	0.844	1.01	134
$n = 64$	0.0104	0.00521	2.24	1.25	761
$n = 128$	0.00503	0.00258	2.1	2.03	$4.37 \cdot 10^{+03}$
$n = 256$	0.00244	0.00123	2.08	2.13	$2.42 \cdot 10^{+04}$
$n = 512$	0.00103	0.000525	2.48	2.46	$1.43 \cdot 10^{+05}$
$n = 1024$	0.00042	0.000213	2.6	2.6	$7.76 \cdot 10^{+05}$
$n = 2048$	0.000135	$6.83 \cdot 10^{-05}$	3.28	3.28	$4.66 \cdot 10^{+06}$

Table C.8: Estimate of the convergence order of the compactly supported sbf φ_7 for testfunction f_1 and parameter $\tau = \pi$

Points	Error L^∞	Error L^2	k_∞	k_2	K_{L^∞}
$n = 16$	0.113	0.0383	6.3	9.41	2.43
$n = 32$	0.0797	0.026	0.997	1.12	6.36
$n = 64$	0.035	0.0172	2.38	1.19	38.6
$n = 128$	0.0167	0.00855	2.13	2.01	208
$n = 256$	0.00819	0.00413	2.05	2.1	$1.14 \cdot 10^{+03}$
$n = 512$	0.0035	0.00178	2.45	2.43	$6.69 \cdot 10^{+03}$
$n = 1024$	0.00144	0.000729	2.57	2.57	$3.61 \cdot 10^{+04}$
$n = 2048$	0.000466	0.000236	3.25	3.25	$2.16 \cdot 10^{+05}$

Table C.9: Estimate of the convergence order of the compactly supported sbf φ_7 for testfunction f_1 and parameter $\tau = \pi/2$

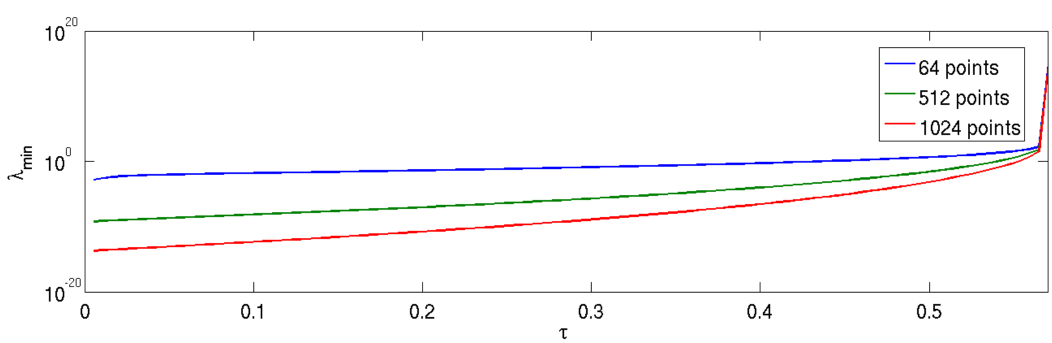

Figure C.1: Minimal eigenvalue of the shifted secans φ_8 interpolation matrix depending on τ when using different point distributions

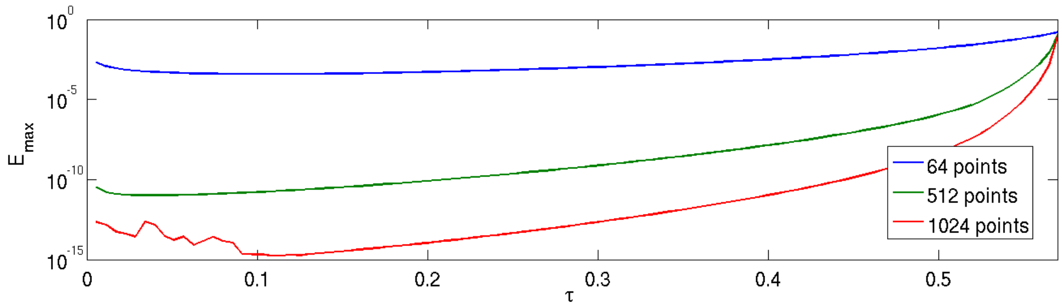

Figure C.2: Maximal error of the shifted secans φ_8 interpolation to testfunction f_1 depending on τ when using different point distributions

Points	Parameter			Error L^∞		
	c_{f_1}	c_{f_2}	c_{f_3}	f_1	f_2	f_3
$n = 16$	0.16	0.108	0.00571	0.0623	0.0131	0.169
$n = 32$	0.00571	0.097	0.00571	0.00823	0.00269	0.00592
$n = 64$	0.103	0.0856	0.00571	0.000386	0.000158	0.000985
$n = 128$	0.097	0.0685	0.00571	$6.33 \cdot 10^{-06}$	$3.48 \cdot 10^{-06}$	$6.06 \cdot 10^{-05}$
$n = 256$	0.0285	0.0571	0.00571	$1.51 \cdot 10^{-08}$	$2.72 \cdot 10^{-08}$	$1.29 \cdot 10^{-07}$
$n = 512$	0.217	0.217	0.217	$1.12 \cdot 10^{-10}$	$4.34 \cdot 10^{-10}$	$1.6 \cdot 10^{-10}$
$n = 1024$	0.405	0.405	0.405	$1.32 \cdot 10^{-11}$	$4.45 \cdot 10^{-10}$	$1.56 \cdot 10^{-10}$

Table C.10: Error minimising values of c for φ_8 with the L^∞ errors of the interpolation of f_1, f_2 and f_3 when condition number is smaller than 10^{10}.

Figure C.1 for $n = 64$, $n = 512$ and $n = 1024$ points. We see that the minimal eigenvalue is smaller for $\tau \to 0$ and for $\tau \to \frac{\pi}{2} - 1$ the minimal eigenvalue tends to infinity. This is the case because the value of the basis function $\varphi_8(1)$, which is the diagonal element of the interpolation matrix, also tends to infinity for $\tau \to \frac{\pi}{2} - 1$.

We also show the corresponding maximum errors of the interpolation of the test function f_1 using φ_8 for the different values of τ. The result is shown in Figure C.2. We again see the trade-off between accuracy and stability, even though for small point numbers the interpolation seems to be more stable than for other basis function. To compare the performance to the other basis functions we choose again an approximate optimal parameter τ which minimises the maximal error while keeping the condition number smaller then 10^{10}. The results are shown in Table C.10.

Appendix D

Remarks on a generalisation of the results of Xu on multiply monotone functions

We want to generalise the results of Yuan Xu which were recently published in [Xu18] to show that the function

$$F_n^{\lambda,\delta}(\theta) = \int_0^\pi (\theta - t)_+^\delta C_n^\lambda(t) \sin(t)^{2\lambda} \, dt > 0, \quad \forall n \in \mathbb{N}, \tag{D.1}$$

is positive definite on $\mathbb{S}^{d-1}$ for $\lambda = \frac{d-2}{2} \leq \delta - 1$. We will here give our advances towards proving the following conjecture, which was also introduced by Gneiting:

Conjecture D.1. *Let $f : \mathbb{R} \to \mathbb{R}$ be a function with compact support* $\operatorname{supp}(f) \subset [0, \pi)$ *that is strictly positive definite as radial basis function on $\mathbb{R}^{d-1}$. Then the restriction of f to $[0, \pi]$ is positive definite on $\mathbb{S}^{d-1}$.*

We will show that the conjecture can be proven by proving Conjecture D.5, which is more specific. To prove the conjecture we will follow the arguments in the article of Xu, which were there used for the function $f(t) = (t - \theta)_+^{\nu-1}$ only. To show the positive definiteness of a general function f we need to compute the Gegenbauer coefficients

$$a_{n,d} := \frac{1}{h_k \lambda} \int_0^\pi f(t) C_n^\lambda(\cos(t)) \left(\sin(t)\right)^{2\lambda} \, dt.$$

Xu used the Jacobi polynomials to define a more general set of expansion coefficients

$$a_n^{\alpha,\beta} := \int_0^\pi f(t) P_n^{\alpha-\frac{1}{2},\beta-\frac{1}{2}}(\cos(t)) \left(\sin(t/2)\right)^{2\alpha} \left(\cos(t/2)\right)^{2\beta} \, dt.$$

They are connected by

$$a_{n,d} = \frac{2^{2\lambda}(2\lambda)_n}{(\lambda+\frac{1}{2})_n} a_n^{\lambda,\lambda},$$

which follows using $C_n^\lambda(t) = \frac{(2\lambda)_n}{(\lambda+\frac{1}{2})_n} P_n^{\lambda-\frac{1}{2},\lambda-\frac{1}{2}}(t)$ for $\lambda > -\frac{1}{2}$, and $\sin(t) = 2\sin(\frac{t}{2})\cos(\frac{t}{2})$.

For progress towards the proof of the conjecture we will need some additional lemmas.

Lemma D.2. *Let $f \in C([0,\pi])$. If $a_n^{\alpha,\beta} \geq 0$ for all $n \in \mathbb{N}$ then $a_n^{\alpha,\beta+1} \geq 0$ for $\beta \geq 0$, $n \in \mathbb{N}$ and the implication also holds true if in both equations the relation is replaced by $>$.*

Proof. We need the following identity from (22.7.16) [AS72]

$$\left(n + \frac{\alpha+\beta}{2} + 1\right)(1+x)P_n^{\alpha,\beta+1}(x) = (n+\beta+1)P_n^{\alpha,\beta}(x) + (n+1)P_{n+1}^{\alpha,\beta}(x),$$

which implies

$$\begin{aligned}\left(\cos\left(\frac{\theta}{2}\right)\right)^2 & P_n^{\alpha-\frac{1}{2},\beta+\frac{1}{2}}(\cos(\theta)) \\ &= \underbrace{\frac{n+\beta+\frac{1}{2}}{2n+\alpha+\beta+1}}_{:=A_n^{\alpha,\beta}>0} P_n^{\alpha-\frac{1}{2},\beta-\frac{1}{2}}(\cos(\theta)) + \underbrace{\frac{n+1}{2n+\alpha+\beta+1}}_{:=B_n^{\alpha,\beta}>0} P_{n+1}^{\alpha-\frac{1}{2},\beta-\frac{1}{2}}(\cos(\theta)).\end{aligned}$$

Therefore we know

$$a_n^{\alpha,\beta+1} = A_{\alpha,\beta} a_n^{\alpha,\beta} + B_n^{\alpha,\beta} a_{n+1}^{\alpha,\beta}.$$

This ends the proof. □

We need one further generalisation of the coefficients

$$\begin{aligned} a_{n,m}^{\alpha,\beta} &= \int_0^\pi f(t) P_{2^m n}^{\alpha-\frac{1}{2},\beta-\frac{1}{2}}(\cos(t/2^m)) \sin(t/2^{m+1})^{2\alpha} \cos(t/2^{m+1})^{2\beta}\, dt \\ &= 2^m \int_0^{\pi/2^m} f(2^m t) P_{2^m n}^{\alpha-\frac{1}{2},\beta-\frac{1}{2}}(\cos(t)) \sin(t/2)^{2\alpha} \cos(t/2)^{2\beta}\, dt. \end{aligned}$$

We can deduce $a_{n,0}^{\alpha,\beta} = a_n^{\alpha,\beta}$.

Lemma D.3. *For $\alpha \geq 0$*

$$a_{n,m}^{\alpha,0} = 2^{2\alpha} \frac{(2^{m+1}n)!(\alpha+\frac{1}{2})_{n2^m}}{(n2^m)!(\alpha+\frac{1}{2})_{2^{m+1}n}} a_{n,m+1}^{\alpha,\alpha}.$$

Proof. From (15.4.15) [AS72] we know that

$$P_{2^m n}^{\alpha-\frac{1}{2},\,-\frac{1}{2}}(\cos(\theta/2^m)) = b_{n,m}^{\alpha} P_{2^{m+1}n}^{\alpha-\frac{1}{2},\alpha-\frac{1}{2}}(\cos(\theta/2^{m+1})),$$

with $b_{n,m}^{\alpha} := \frac{(2^{m+1}n)!(\alpha+\frac{1}{2})_{2^m n}}{(2^m n)!(\alpha+\frac{1}{2})_{2^{m+1}n}}$. We also use the equality $\sin\theta = 2\sin(\theta/2)\cos(\theta/2)$ from which it follows that

$$\begin{aligned}
a_{n,m}^{\alpha,0} &= \int_0^{\pi} f(t) P_{2^m n}^{\alpha-\frac{1}{2},-\frac{1}{2}}(\cos(t/2^m)) \sin(t/2^{m+1})^{2\alpha}\, dt \\
&= b_{n,m}^{\alpha} 2^{2\alpha} \int_0^{\pi} f(t) P_{2^{m+1}n}^{\alpha-\frac{1}{2},\alpha-\frac{1}{2}}(\cos(t/2^{m+1})) \sin(t/2^{m+2})^{2\alpha} \cos(t/2^{m+2})^{2\alpha}\, dt \\
&= b_n^{\alpha} 2^{2\alpha} a_{n,m+1}^{\alpha,\alpha}.
\end{aligned}$$

□

This shows that $a_{n,m}^{\alpha,0} > 0 \Leftrightarrow a_{n,m+1}^{\alpha,\alpha} > 0$. We will now apply a property of the Jacobi polynomials stated in (22.15.1), [AS72]:

$$\lim_{m\to\infty} m^{-\alpha} P_m^{\alpha,\beta}(\cos(z/m)) = \left(\frac{z}{2}\right)^{-\alpha} J_{\alpha}(z),$$

uniformly in every bounded region of the complex plane.

To prove the conjecture we also need to show that the coefficients are summable. To do so we follow in parts the arguments of Beatson et al. [BzCX14] who showed the convergence for (D.1). We cite from [BzCX14] Lemma 3.1 without proof.

Lemma D.4. *For $\mu \geq 1$, it is true that*

$$C_n^{\mu}(\cos(\theta)\,(\sin(\theta))^{2\mu} = \sum_{k=0}^{\infty} c_{k,n}^{\mu} \cos\left((n+2k)\theta\right), \tag{D.2}$$

where

$$c_{k,n}^{\mu} := \frac{2^{1-2\mu}(-\mu)_k \Gamma(n+2\mu)\Gamma(n+k)(n+2k)}{\Gamma(\mu) n! k! \Gamma(n+k+\mu+1)}.$$

When $\mu \in \mathbb{N}$, then the summation terminates at $k = \mu$ and the expression for $c_{k,n}^{\mu}$ can be rewritten as

$$c_{k,n}^{\mu} = \frac{2^{1-2\mu}}{\Gamma(\mu)}(-1)^k \binom{\mu}{k} \frac{(n+1)_{2\mu-1}(n+2k)}{(n+k)_{\mu+1}}.$$

Conjecture D.5. *Let $f \in C([0,\pi])$. If $a_{n,m}^{\alpha,\beta} \geq 0$ for all $n \in \mathbb{N}$ then $a_{n,m}^{\alpha,\beta+1} \geq 0$ for $\beta \geq 0$ and the implication also holds true if in both equations the relation is replaced by $>$.*

Theorem D.6. *If Conjecture D.5 is true then the functions in Conjecture D.1 have only positive Gegenbauer coefficients.*

Proof. Since $\lambda > 0$ we set $\alpha = \lambda > 0$. To show $a_n^{\alpha,\beta} > 0$ for all β using Lemma D.2 it is enough to show $a_n^{\alpha,0} > 0$. Using the previous results we know already

$$a_{n,m}^{\alpha,0} = 2^{2\alpha} b_n^{\alpha} a_{n,m+1}^{\alpha,\alpha}.$$

Since we suppose Conjecture D.5 to be true, this can be repeatedly applied since the proof of

$$a_{n,j}^{\alpha,0} > 0$$

for any $j \in \mathbb{N}$ implies $a_{n,0}^{\alpha,\alpha} > 0$. We now use the result on the limit by [Sze39] Theorem 8.1 of the Jacobi polynomials together with the linear approximation of the sin near zero

$$\begin{aligned}\lim_{j\to\infty} 2^{j(\alpha+\frac{1}{2})} P_{2^j n}^{\alpha-\frac{1}{2},-\frac{1}{2}}(\cos(t/2^j))\left(\sin(t/2^j)\right)^{2\alpha} &= n^{\alpha-\frac{1}{2}} t^{2\alpha} \lim_{j\to\infty} \frac{P_{2^j n}^{\alpha-\frac{1}{2},\frac{1}{2}}(\cos(t/2^j))}{(2^j n)^{\alpha-\frac{1}{2}}} \\ &= 2^{\alpha-\frac{1}{2}} t^{\alpha+\frac{1}{2}} J_{\alpha-\frac{1}{2}}(nt).\end{aligned}$$

This can now be applied for the computation of

$$\lim_{j\to\infty} 2^{j(\alpha+\frac{1}{2})} a_{2^j n,j}^{\alpha,0}(t) = \int_0^{\pi} f(t)(2)^{\alpha-\frac{1}{2}} t^{\alpha+\frac{1}{2}} J_{\alpha-\frac{1}{2}}(nt)\, dt.$$

The positivity of the coefficients now follows because

$$\int_0^{\pi} f(t)(2)^{\alpha-\frac{1}{2}} t^{\alpha+\frac{1}{2}} J_{\alpha-\frac{1}{2}}(nt)\, dt = n^{\frac{d-1}{2}} F_{d-1} f(\xi) > 0 \tag{D.3}$$

for any $\xi \in \mathbb{R}^d$ with $\|\xi\| = n$, and $F_{d-1} f$ the $(d-1)$-dimensional Fourier transform of f. This is positive because of Bochner's theorem. □

To show the convergence of the sum of the coefficients is still an open problem but we believe to be able to solve it using the results of R. Beatson et al.. Suppose $\lambda \in \mathbb{N}$

and apply (D.2)

$$\begin{aligned}
a_{n,d} &= \int_0^\pi f(t) C_n^\lambda(\cos(t)) \left(\sin(t)\right)^{2\lambda}\, dt \\
&= \int_0^\pi f(t) \sum_{k=0}^{\infty} c_{k,n}^\lambda \cos\left((n+2k)t\right)\, dt \\
&= \int_0^\pi f(t) \sum_{k=0}^{\lambda} (-1)^k \frac{2^{1-2\lambda}}{\Gamma(\lambda)} \binom{\lambda}{k} \frac{(n+1)_{2\lambda-1}(n+2k)}{(n+k)_{\lambda+1}} \cos\left((n+2k)t\right)\, dt \\
&= \sum_{k=0}^{\lambda} \underbrace{(-1)^k \frac{2^{1-2\lambda}}{\Gamma(\lambda)} \binom{\lambda}{k} \frac{(n+1)_{2\lambda-1}(n+2k)}{(n+k)_{\lambda+1}}}_{=\mathcal{O}(n^{\lambda-1})} \underbrace{\int_0^\pi f(t) \cos\left((n+2k)t\right)\, dt}_{\tilde{f}(n+2k)},
\end{aligned}$$

where $\tilde{f}(n)$ are the Fourier coefficients of the even extension of f to the interval $[-\pi, \pi]$. To show $\sum_{n=0}^{\infty} a_n^\lambda < \infty$ it is sufficient to prove $\tilde{f}(n) = \mathcal{O}(n^{-(\lambda+2)})$. We hope that in the near future we will be able to prove Conjecture D.1 employing the findings of this thesis.

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Number Sets

$\mathbb{N}_m$	The natural numbers greater than or equal to m
$\mathbb{R}$, $\mathbb{R}_{>0}$, $\mathbb{R}_{\geq 0}$	The real numbers, the positive and non-negative reals
$\mathbb{R}^d$	The real vectors of dimension d
$\mathbb{Z}$	The integers
$\mathbb{Z}^n$	Multi-index of n-integers

Function Spaces

H_φ, $\|\cdot\|_\varphi$	The native Hilbert space of a spherical basis function φ and the corresponding norm
$\overline{\mathbb{P}}_k^d$	Space of tensor product polynomials of d variables and degree at most k
$\mathbb{P}_m^d$	The polynomials in d variables of total degree at most m
$C^k(I)$, $C^\infty(I)$	The function class of k-times differentiable functions on I or arbitrary often differentiable functions on I
$CSPD_m(\mathbb{S}^{d-1})$, $SPD(\mathbb{S}^{d-1})$	Spaces of (conditionally) strictly positive definite functions on the $d-1$ dimensional sphere
$H_k^*(\mathbb{S}^{d-1})$, $N_{d,k}$	Space of spherical harmonics of degree k on the $d-1$ dimensional sphere, dimension of this space
$H_k^+(\mathbb{S}^{d-1})$	Space of spherical harmonics of degree smaller or equal to k on the $d-1$ dimensional sphere

$L^1(I)$, $L^2(I)$	The function class of absolutely or square integrable functions on I
$S(\mathbb{R}^d)$	Schwartz space on $\mathbb{R}^d$
$W_2^\beta(\mathbb{S}^{d-1})$	Sobolev space on the $(d-1)$-dimensional sphere

Functions

$\Gamma_q(x)$	q-Gamma functions
$\hat{f}$	Fourier transform of the function f
Φ	Radial basis function of the form $\mathbb{R}^d \to \mathbb{R}$
ϕ	Radial basis function of the form $\mathbb{R}_{\geq 0} \to \mathbb{R}$
ϕ_c	Shifted radial basis functions
C_k^λ, λ	Gegenbauer polynomials, usually $\lambda = \frac{d-2}{2}$
J_τ	Bessel function of the first kind
$K_\tau(x)$	modified Bessel functions
$P_{\varphi,\gamma*}$	Optimal powerfunction
s	Interpolant or approximant
s_f	φ-based interpolant to function f

Other Symbols

$\hat{\varphi}(j)$	Fourier coefficient of a spherical basis function φ
$\hat{f}_{j,\ell}$	Coefficients of the spherical harmonic decomposition of $f \in L^2(\mathbb{S}^{d-1})$
λ_k	Eigenvalues of the Laplace-Beltrami operator on the sphere
$\mathbb{S}^{d-1}$	The unit sphere of dimension $d-1$
$\mathcal{R}x$	Real part of x
ω_d, $d\omega_{\mathbb{S}^{d-1}}$	Surface area and surface measure of the sphere $\mathbb{S}^{d-1}$

$\triangle^*_{d-1}$	The Laplace-Beltrami operator on the sphere
$\triangle_d$	The Laplace operator
$\|x\|$	The Euclidean norm of the vector $x \in \mathbb{R}^d$
Ξ	Distinct and finite set of data sites, subset of $\mathbb{R}^d$ or $\mathbb{S}^{d-1}$
A_Ξ	Interpolation matrix
$a_{k,d}$	Gegenbauer coefficients of a spherical basis function
$d(\cdot,\cdot)$	Geodesic distance between two points on a unit sphere
h_k^λ	Constant used in the computation of the Gegenbauer coefficients
h_ξ	Geodesic mesh distance of a set $\Xi \subset \mathbb{S}^{d-1}$

Bibliography

[AS72] M. Abramowitz and I. A. Stegun. *Handbook of mathematical functions.* Dover Publications, Inc., New York, 1972.

[Ask75] R. Askey. Some characteristic functions of unimodal distributions. *Journal of Mathematical Analysis and Applications*, 50:465 – 469, 1975.

[BCM$^+$06] L. Bos, M. Caliari, S. De Marchi, M. Vianello, and Y. Xu. Bivariate Lagrange interpolation at the Padua points: The generating curve approach. *Journal of Approximation Theory*, 143:15 – 25, 2006. Special Issue on Foundations of Computational Mathematics.

[Bin73] N. H. Bingham. Positive definite functions on spheres. In *Mathematical Proceedings of the Cambridge Philosophical Society*, pages 145–156. Cambridge University Press, 1973.

[BLM11] R. K. Beatson, J. Levesley, and C. T. Mouat. Better bases for radial basis function interpolation problems. *Journal of Computational and Applied Mathematics*, 236:434 – 446, 2011.

[BM91] M. D. Buhmann and C. A. Micchelli. Multiply monotone functions for cardinal interpolation. *Advances in Applied Mathematics*, 12:358–386, 1991.

[BM13] J. P. Boyd and P. W. McCauley. Quartic Gaussian and inverse-quartic Gaussian radial basis functions: The importance of a nonnegative Fourier transform. *Computers & Mathematics with Applications*, 65:75–88, 2013.

[Boy14] J. P. Boyd. The Fourier transform of the quartic Gaussian $exp(-ax4)$: Hypergeometric functions, power series, steepest descent asymptotics and hyperasymptotics and extensions to $exp(-ax2n)$. *Applied Mathematics and Computation*, 241:75–87, 2014.

[Buh90] M. D. Buhmann. Multivariate cardinal interpolation with radial-basis functions. *Constructive Approximation*, 6:225–255, 1990.

[Buh03] M. D. Buhmann. *Radial Basis Functions*. Cambridge University Press, Cambridge, 2003.

[BzC17] R. K. Beatson and W. zu Castell. Dimension hopping and families of strictly positive definite zonal basis functions on spheres. *Journal of Approximation Theory*, 221:22 – 37, 2017.

[BzCX14] R. K. Beatson, W. zu Castell, and Y. Xu. A Pólya criterion for (strict) positive-definiteness on the sphere. *IMA Journal of Numerical Analysis*, 34:550–568, 2014.

[Cat99] F. S. Cater. On monotonic and analytic functions in C^∞. *Real Analysis Exchange*, 23:697–708, 1999.

[dB90] C. de Boor. *Splinefunktionen*. Birkhäuser, 1990.

[dB01] C. de Boor. *A practical guide to splines; rev. ed.* Applied mathematical sciences. Springer, Berlin, 2001.

[Des04] M. Deserno. How to generate equidistributed points on the surface of a sphere. *P.-If Polymerforshung (Ed.)*, page 99, 2004.

[DF02] T. A. Driscoll and B. Fornberg. Interpolation in the limit of increasingly flat radial basis functions. *Computers & Mathematics with Applications*, 43:413–422, 2002.

[DL93] R. A. DeVore and G. G. Lorentz. *Constructive Approximation*. Springer-Verlag, 1993.

[DNW97] N. Dyn, F. J. Narcowich, and J. D. Ward. A framework for interpolation and approximation on Riemannian manifolds. *Approximation Theory and Optimization: Tributes to MJD Powell*, pages 133–144, 1997.

[DNW99] N. Dyn, F. J. Narcowich, and J. D. Ward. Variational principles and Sobolev-type estimates for generalized interpolation on Riemannian manifolds. *Constructive Approximation*, 15:175–208, 1999.

[DNZ99] O. Davydov, G. Nürnberger, and F. Zeilfelder. Interpolation by splines on triangulations. In *New Developments in Approximation Theory*, pages 49–70. Springer, 1999.

[Fas07] G. E. Fasshauer. *Meshfree Approximation Methods with MATLAB*, volume 6 of *Interdisciplinary mathematical sciences*. World Scientific Publishing Co. Pte. Ltd., 2007.

[FLW06] B. Fornberg, E. Larsson, and G. Wright. A new class of oscillatory radial basis functions. *Computers & Mathematics with Applications*, 51:1209 – 1222, 2006.

[Fly06] N. Flyer. Exact polynomial reproduction for oscillatory radial basis functions on infinite lattices. *Computers & Mathematics with Applications*, 51:1199 – 1208, 2006.

[Fra82] R. Franke. Scattered data interpolation: Tests of some methods. *Mathematics of Computation*, 38:181–200, 1982.

[FWL04] B. Fornberg, G. Wright, and E. Larsson. Some observations regarding interpolants in the limit of flat radial basis functions. *Computers & Mathematics with Applications*, 47:37–55, 2004.

[GHS93] K. Guo, S. Hu, and X. Sun. Conditionally positive definite functions and Laplace-Stieltjes integrals. *Journal of Approximation Theory*, 74:249–265, 1993.

[Gne13] T. Gneiting. Strictly and non-strictly positive definite functions on spheres. *Bernoulli*, 19:1327–1349, 2013.

[GQ10] B. Guo and F. Qi. A property of logarithmically absolutely monotonic functions and the logarithmically complete monotonicity of a power-exponential function. *Politehn. Univ. Bucharest Sci. Bull. Ser. A Appl. Math. Phys*, 72:21–30, 2010.

[GR14] I. S. Gradshteyn and I. M. Ryzhik. *Table of integrals, series, and products.* Academic press, 2014.

[GS00] Mariano Gasca and Thomas Sauer. Polynomial interpolation in several variables. *Advances in Computational Mathematics*, 12:377–417, 2000.

[Guo16] S. Guo. On completely monotonic and related functions. *Filomat*, 30:2083–2090, 2016.

[Hak82] H. A. Hakopian. Multivariate divided differences and multivariate interpolation of Lagrange and Hermite type. *Journal of Approximation Theory*, 34:286 – 305, 1982.

[Har90] R. L. Hardy. Theory and applications of the multiquadric-biharmonic method. *Computers Math. Applic.*, 19:163–208, 1990.

[HB01] S. Hubbert and B. Baxter. Radial basis functions for the sphere. *Recent Progress in Multivariate Approximation*, 137:33–47, 2001.

[HH13] K. Höllig and J. Hörner. *Approximation and Modelling with Splines*. Society for Industrial and applied Mathematics, 2013.

[HLGM15] S. Hubbert, Q. T. Lê Gia, and T. M. Morton. *Spherical radial basis functions, theory and applications*. Springer, 2015.

[HM04a] S. Hubbert and T. M. Morton. l_p-error estimates for radial basis function interpolation on the sphere. *Journal of Approximation Theory*, 129:58–77, 2004.

[HM04b] S. Hubbert and T. M. Morton. On the accuracy of surface spline interpolation on the unit sphere. *Advances in Constructive Approximation: Vanderbild 2003*, pages 227–242, 2004.

[Hof13] R. Hofmann. Neue Verfahren zur Approximation mit radialen Basisfunktionen und numerische Untersuchung der Dagum-Funktionen. *Dissertation Universität Giessen*, 2013.

[Hub02] S. Hubbert. Radial basis functions interpolation on the sphere. *Dissertation Imperial College London*, 2002.

[Jäg14] J. Jäger. Rekonstruktion von EEG Daten mittels radialer Basisfunktionen. *Masterarbeit Justus Liebig-Universität Giessen*, 2014.

[JKBS16] J. Jäger, A. Klein, M. Buhmann, and W. Skrandies. Reconstruction of electroencephalographic data using radial basis functions. *Clinical Neurophysiology*, 127:1978–1983, 2016.

[Joh98] M. J. Johnson. A bound on the approximation order of surface splines. *Constructive Approximation*, 14:429–438, 1998.

[JSW99] K. Jetter, J. Stöckler, and J. Ward. Error estimates for scattered data interpolation on spheres. *Mathematics of Computation, American Mathematical Society*, 68:733–747, 1999.

[Ker80] P. Kergin. A natural interpolation of C^k functions. *Journal of Approximation Theory*, 29:278 – 293, 1980.

[KM18] J. E. Kamel and K. Mehrez. A function class of strictly positive definite and logarithmically completely monotonic functions related to the modified Bessel functions. Positivity, 2018. Online at `https://doi.org/10.1007/s11117-018-0584-3`.

[Lev98] D. Levin. The approximation power of moving least-squares. *Mathematics of Computation, American Mathematical Society*, 67:1517–1531, 1998.

[LLRS99] J. Levesley, W. Light, D. Ragozin, and X. Sun. A simple approach to the variational theory for interpolation on spheres. In *New Developments in Approximation Theory*, pages 117–143. Springer, 1999.

[LMS70] L. Lorch, M. E. Muldoon, and P. Szegő. Higher monotonicity properties of certain Sturm-Liouville functions. iii. *Canad. J. Math*, 22:1238–1265, 1970.

[LN83] L. Lorch and D. J. Newman. On the composition of completely monotonic functions and completely monotonic sequences and related questions. *Journal of the London Mathematical Society*, 28:31–45, 1983.

[Mai56] J. C. Mairhuber. On Haar's theorem concerning Chebychev approximation problems having unique solutions. *Proceedings of the American Mathematical Society*, 7:609–615, 1956.

[MB02] C. T. Mouat and R. K. Beatson. Rbf collocation. *Research report UCDMS 2002/3*, 2002.

[McH75] J. A. M. McHugh. A proof of Bernstein's theorem on regularly monotonic functions. In *Proceedings of The American Mathematical Society*, volume 47, pages 158–360. 1975.

[Meh15] K. Mehrez. Logarithmically completely monotontic functions related the $q-$ gamma and the $q-$ digamma functions with applications. *arXiv preprint arXiv:1511.07156*, 2015.

[Men94] V. A. Menegatto. Strictly positive definite kernels on the Hilbert sphere. *Applicable Analysis*, 55:91–101, 1994.

[Men04] V. A. Menegatto. Conditionally positive definite kernels on Euclidean domains. *Journal of Mathematical Analysis and Applications*, 294:345 – 359, 2004.

[Mic86] C. A. Micchelli. Interpolation of scattered data: Distance matrices and conditionally positive definite functions. *Constructive Approximation*, 2:11–22, 1986.

[MM80] C. A. Micchelli and P. Milman. A formula for Kergin interpolation in R^k. *Journal of Approximation Theory*, 29:294–296, 1980.

[Mon11] M. Mongillo. Choosing basis functions and shape parameters for radial basis function methods. *SIAM Undergraduate research online*, 4, 2011.

[Mue66] C. Mueller. Spherical harmonics. *Springer Lecture Notes in Mathematics*, 17, 1966.

[NSW07] F. J. Narcowich, X. Sun, and J. D. Ward. Approximation power of RBFs and their associated SBFs: a connection. *Advances in Computational Mathematics*, 27:107–124, 2007.

[NW02] F. Narcowich and J. Ward. Scattered data interpolation on spheres: Error estimates and locally supported basis functions. *SIAM Journal on Mathematical Analysis*, 33:1393–1410, 2002.

[OOL+18] F. W. J. Olver, A. B. Olde Daalhuis, D. W. Lozier, B. I. Schneider, R. F. Boisvert, C. W. Clark, B. R. Miller, and eds. B. V. Saunders. *NIST Digital Library of Mathematical Functions.* http://dlmf.nist.gov/, Release 1.0.15 of 2017-06-01, 2018.

[Qi05] F. Qi. Certain logarithmically n-alternating monotonic functions involving gamma and q-gamma functions. *RGMIA Res. Rep. Coll.*, 8, 2005.

[Rip99] S. Rippa. An algorithm for selecting a good value for the parameter c in radial basis function interpolation. *Advances in Computational Mathematics*, 11:193–210, 1999.

[Ron92] A. Ron. Principal shift-invariante spaces. *Numerical Methods in Approximation Theory*, 9:221–244, 1992.

[Sch38] I. J. Schoenberg. Metric spaces and positive definite functions. *Transactions of the American Mathematical Society*, 44:522–536, 1938.

[Sch42] I. J. Schoenberg. Positive definite functions on the sphere. *Duke Math. J.*, 9:96–108, 1942.

[Sch99] R. Schaback. Native Hilbert spaces for radial basis functions I. In *New Developments in Approximation Theory*, pages 255–282. Springer, 1999.

[Sch15] L. Schumaker. *Spline Functions computational methods*. Society for Industrial and Applied Mathematics Philadelphia, 2015.

[SL16] V. Shcherbakov and E. Larsson. Radial basis function partition of unity methods for pricing vanilla basket options. *Computers & Mathematics with Applications*, 71:185 – 200, 2016.

[STRL+91] L. Soufflet, M. Toussaint, R-Luthringer, J. Gresser, R. Minot, and J. P. Macher. A statistical evaluation of the main interpolation methods to 3-dimensional EEG mapping. *Electroencephalography and clinical Neurophysiology*, 79:393–402, 1991.

[SW01] R. Schaback and H. Wendland. Characterization and construction of radial basis functions. *Multivariate Approximation and Applications*, pages 1–25, 2001.

[Sze39] G. Szegő. *Orthogonal polynomials*, volume 23. American Mathematical Soc., 1939.

[vH96] H. van Haeringen. Completely monotonic and related functions. *Journal of Mathematical Analysis and Applications*, 204:389 – 408, 1996.

[Wen96] H. Wendland. Konstruktion und Untersuchung radialer Basisfunktionen mit kompaktem Träger. *Dissertation Universität Göttingen*, 1996.

[Wen05] H. Wendland. *Scattered Data Approximation*. Cambridge University Press, 2005.

[Wid46] D. V. Widder. *The Laplace Transform*. Princeton University Press, 1946.

[Wil56] R. E. Williamson. Multiply monotone functions and their Laplace transforms. *Duke Mathematical Journal*, 23:189–207, 1956.

[Wü13] B. Würzer. *Visuell evozierte Potentiale und ihre Topographie beim Lernen japanischer Symbole unter Geruchseinflüssen*. Gießen, 2013. MD thesis.

[XC92] Y. Xu and E. W. Cheney. Strictly positive definite functions on spheres. *Proc. of the American mathematical society*, 116:977–981, 1992.

[Xu18] Y. Xu. Positive definite functions on the unit sphere and integrals of Jacobi polynomials. *Proc. of the American mathematical society*, 146:2039–2048, 2018.

[zCF04] W. zu Castell and F. Filbir. Radial basis functions and corresponding zonal series expansions on the sphere. *Journal of Approximation Theory*, 134:65–79, 2004.

[ZP17] V. P. Zastavnyi and E. Porcu. On positive definiteness of some radial functions. *Lobachevskii Journal of Mathematics*, 38:386–394, 2017.

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