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Radial basis functions and corresponding zonal series expansions on the sphere

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Abstract

Since radial positive definite functions on $\mathbb{R}^d$ remain positive definite when restricted to the sphere, it is natural to ask for properties of the zonal series expansion of such functions which relate to properties of the Fourier–Bessel transform of the radial function. We show that the decay of the Gegenbauer coefficients is determined by the behavior of the Fourier–Bessel transform at the origin.

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1. Introduction

Approximating functions by linear combinations of translates of a single basis function is a widely used method in several branches of mathematics. Methods of this kind are *radial basis function methods* in approximation theory and *kriging methods* in multivariate statistics. There is a large literature on the subject in both areas of mathematics (cf. [3,19], and the references therein). Given a function $\phi : \mathbb{R}_+ \to \mathbb{R}$ and data $X = \{(\mathbf{x}_1, f_1), \ldots, (\mathbf{x}_N, f_N)\} \subset \mathbb{R}^d \times \mathbb{R}$, the basic idea of radial basis function interpolation is

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to assume the values $f_1, \ldots, f_N$ to be point evaluations of an unknown function $f : \mathbb{R}^d \to \mathbb{R}$, and to recover *f* from a linear combination of the type

$$s_{f,X}(\mathbf{y}) = \sum_{j=1}^{N} a_j \phi(|\mathbf{y} - \mathbf{x}_j|), \qquad \mathbf{y} \in \mathbb{R}^d.$$

Since the *basis function* $\phi(|\cdot|)$ depends on the norm of the argument only, it is called *radial*. A natural class of suitable basis functions is the class of *positive definite radial* functions. These are continuous functions $\phi : \mathbb{R}^d \to \mathbb{R}$, such that for all finite sets of points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ and arbitrary coefficients $c_1, \ldots, c_n \in \mathbb{C}$ the inequality

$$\sum_{j=1}^{n} \sum_{k=1}^{n} \overline{c}_j c_k \phi(|\mathbf{x}_j - \mathbf{x}_k|) \geqslant 0 \tag{1.1}$$

holds true. Note that the common definition of positive definite functions does in general not include continuity of the function. But in the context of radial basis function interpolation this is a reasonable assumption.

There is an analogous concept for radial basis functions on the unit sphere $\mathbb{S}^{d-1}$ in $\mathbb{R}^d$. We then assume the basis function ψ to depend on the geodesic distance of two points on the sphere, only, and define positive definiteness in an analog manner. One can show (cf. [18, (1.3)]) that these functions can be represented as a *zonal series*,

$$\psi(\xi, \eta) = \sum_{n=0}^{\infty} d_n \sum_{k=1}^{c_{n,d}} S_{n,k}(\xi) S_{n,k}(\eta), \qquad \xi, \eta \in \mathbb{S}^{d-1}, \tag{1.2}$$

where $\{S_{n,k} : 1 \leqslant k \leqslant c_{n,d}\}$ denotes a basis of the space of spherical harmonics (cf. (2.11), below).

Many results for radial basis functions on $\mathbb{R}^d$ have their counterparts on the sphere (cf. for example [7]). One difficulty with the so-called *zonal basis function* approach is to find suitable basis functions on the sphere. Since the restriction of a positive definite function on $\mathbb{R}^d$ to the sphere is positive definite on $\mathbb{S}^{d-1}$, it is natural to ask which properties of the radial basis functions can be naturally transferred to the sphere.

Comparing Fourier transform and zonal series expansion for several examples of known basis functions (see e.g., [11]). Levesley and Hubbert [12] came up with the following conjecture.

Conjecture A. *Let* ϕ *be radial on* $\mathbb{R}^d$ *such that for some* $k \in \mathbb{N}$ *the function* $(-1)^k \phi^{(k)}$ *is completely monotone on* $(0, \infty)$. *Let further the generalized Fourier transform of* ϕ *have polynomial decay, i.e.,*

$$\widehat{\phi}(t) = \mathcal{O}(t^{-d-\alpha})$$

for some $\alpha > 0$, *and*

$$\psi(\xi,\eta) = \sum_{n=0}^{\infty} d_n \sum_{k=1}^{c_{n,d}} S_{n,k}(\xi) S_{n,k}(\eta), \qquad \xi,\eta \in \mathbb{S}^{d-1},$$

denotes the zonal series expansion of the restriction of ϕ *to the sphere, i.e.,*

$$\psi(\xi,\eta) = \phi\left(\sqrt{2-2\xi^t\eta}\right), \qquad \xi,\eta \in \mathbb{S}^{d-1}.$$

Then the Fourier coefficients $\{d_n\}$ *have an analog decay rate. To be precise,*

$$d_n = \mathcal{O}(n^{-d-\alpha+1}), \quad \textit{as } n \to \infty.$$

The aim of the present paper is to analyze the conjecture in some detail and to give a proof of a clarified version of it. The basic idea is to use properties of the underlying systems of special functions to bridge the gap between the Fourier transform $\widehat{\phi}$ and the zonal series coefficients d_n.

To keep the paper self-contained, we summarize the important definitions and properties in the next paragraph and discuss several aspects of the conjecture. At the end we will put the conjecture into a form which can be proved. We will give the proof for the special case that ϕ is positive definite in Section 3. Section 4 then deals with the general case. The last section finally gives some remarks on the underlying concepts, trying to provide some understanding of the concept of smoothness and radial/zonal functions.

2. Prerequisites

Before analyzing the conjecture let us collect some basic facts on Fourier transforms and special functions. By $\mathcal{S}(\mathbb{R}^d)$ we denote the Schwarz space on $\mathbb{R}^d$, i.e., the space of functions $\varphi \in C^{\infty}(\mathbb{R}^d)$ with $\sup_{\mathbf{x}\in\mathbb{R}^d} |\mathbf{x}^m \partial^n \varphi(\mathbf{x})| < \infty$ for all $n, m \in \mathbb{N}_0^d$. A function $\phi \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ is called of polynomial growth if there is an $\ell \in \mathbb{N}_0$ such that $|\phi(\mathbf{x})| = \mathcal{O}(|\mathbf{x}|^{\ell})$ for $|\mathbf{x}| \to \infty$. Such functions can be considered as generalized functions on $\mathcal{S}(\mathbb{R}^d)$ in the usual way. The *generalized Fourier transform* for such functions is then defined as

$$\int_{\mathbb{R}^d} \widehat{\phi}(\mathbf{x})\varphi(\mathbf{x})\, d\mathbf{x} = \int_{\mathbb{R}^d} \phi(\mathbf{x})\widehat{\varphi}(\mathbf{x})\, d\mathbf{x} \tag{2.1}$$

for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$.

Recall, the *Bessel function* of the first kind and of order $\nu > -\frac{1}{2}$ is defined by its power series

$$J_\nu(z) = \frac{1}{\Gamma(\nu+1)}\left(\frac{z}{2}\right)^{\nu} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\,\Gamma(\nu+k+1)}\left(\frac{z}{2}\right)^{2k}, \qquad z \in \mathbb{C}. \tag{2.2}$$

Since it is sometimes more convenient, let us also introduce a second commonly used notation:

$$\mathcal{J}_\nu(z) = \Gamma(\nu+1)\left(\frac{z}{2}\right)^{-\nu} J_\nu(z), \qquad z \in \mathbb{C}.$$

The Fourier–Bessel transform of a radial function on $\mathbb{R}^d$ is defined as (cf. [17])

$$\widehat{\phi_0}(t) = k_\lambda \int_0^\infty \phi_0(r)\mathcal{J}_\lambda(rt)r^{2\lambda+1}\,dr, \qquad t \in \mathbb{R}_+, \tag{2.3}$$

where $k_\lambda = (2^\lambda \Gamma(\lambda+1))^{-1}$. Here and for the rest of the paper λ denotes the fixed parameter $\lambda = \frac{d-2}{2}$. The constant k_λ is chosen such that the transform is self-inverse, i.e., $\widehat{\widehat{\phi}}_0(r) = \phi_0(r)$, for suitable functions ϕ_0. The function ϕ_0 thereby denotes the radial function ϕ considered as a function on the positive real line.

In case of a radial function ϕ Eq. (2.1) reads

$$k_\lambda \int_0^\infty \widehat{\phi_0}(r)\varphi(r)r^{2\lambda+1}\,dr = k_\lambda \int_0^\infty \phi_0(r)\widehat{\varphi}(r)r^{2\lambda+1}\,dr \tag{2.4}$$

for all $\varphi \in \mathcal{S}(\mathbb{R}_+)$.

Let $\phi \in L^1_{\text{loc}}(\mathbb{R}^d)$ be a function of polynomial growth. Then ϕ is a *generalized positive definite function* on $\mathcal{S}(\mathbb{R}^d)$ if and only if it can be represented as

$$\int_{\mathbb{R}^d} \phi(\mathbf{x})\varphi(\mathbf{x})\,d\mathbf{x} = \int_{\mathbb{R}^d} \widehat{\varphi}(\mathbf{x})\,d\mu(\mathbf{x}), \tag{2.5}$$

where μ is a positive tempered measure, i.e., a positive measure which additionally satisfies

$$\int_{\mathbb{R}^d} (1+|\mathbf{x}|^2)^{-p}\,d\mu(\mathbf{x}) < \infty$$

for some $p \geqslant 0$ (see, e.g., [8]). Using (2.5) and the Fourier–Bessel transform (2.3), we obtain the following representation for a radial positive definite function:

$$\phi_0(r) = k_\lambda \int_0^\infty \mathcal{J}_\lambda(rt)t^{2\lambda+1}\,d\mu(t), \qquad r \in \mathbb{R}_+, \tag{2.6}$$

where μ is a positive tempered measure on $\mathbb{R}_+$. Since we are dealing with radial functions only, we will identify the radial functions on $\mathbb{R}^d$ with their counterparts on $\mathbb{R}_+$, thus, skipping the subscript. Likewise, the notation $\widehat{\phi}$ has to be interpreted accordingly.

Let us finally recall some important facts about Gegenbauer polynomials and their connection to Bessel functions. The *Gegenbauer polynomials* of degree $n \in \mathbb{N}$ with parameter $\nu > 0$ can be defined using their generating function

$$(1 - 2r\cos\theta + r^2)^{-\nu} = \sum_{n=0}^\infty r^n C_n^\nu(\cos\theta), \qquad \theta \in [0,\pi]. \tag{2.7}$$

Gegenbauer polynomials are orthogonal on the interval $[0, \pi]$ with respect to the measure $\sin^{2v}\,\theta\, d\theta$ and are normalized such that

$$|C_n^v(\cos\theta)| \leqslant C_n^v(1) = \frac{(2v)_n}{n!}, \qquad \theta \in [0, \pi]. \tag{2.8}$$

There is an important connection between Gegenbauer polynomials and Bessel functions of order $v > -\frac{1}{2}$, known as *Gegenbauer's addition theorem* for Bessel functions:

$$\frac{J_v(c)}{c^v} = 2^v \Gamma(v) \sum_{n=0}^{\infty} (v+n) \frac{J_{v+n}(a)}{a^v} \frac{J_{v+n}(b)}{b^v} C_n^v(\cos\,\theta), \tag{2.9}$$

where a, b, c are the lengths of the sides of a triangle, and θ is the angle between the sides of length a and b, respectively.

In [18] Schoenberg proved that a function f on $\mathbb{S}^{d-1}$ is positive definite if and only if f has a Gegenbauer expansion

$$f(\xi^t \eta) = \sum_{n=0}^{\infty} a_n C_n^{\lambda}(\cos\,\theta), \qquad \xi, \eta \in \mathbb{S}^{d-1}, \tag{2.10}$$

with non-negative coefficients $a_n \in \mathbb{R}$, $n \in \mathbb{N}_0$, and $\theta = \arccos\, \xi^t \eta$.

To explain the connection between Gegenbauer polynomials and functions on the sphere, we have to introduce spherical harmonics. For further details on spherical harmonics the reader is referred to the monograph [15].

The space $C(\mathbb{S}^{d-1})$ of real-valued continuous functions on the sphere in $\mathbb{R}^d$ can be decomposed into the direct sum of spaces of harmonic polynomials on the sphere in d variables, i.e.,

$$C(\mathbb{S}^{d-1}) = \bigoplus_{n=0}^{\infty} \mathcal{H}_d^n.$$

There is an inner product on $C(\mathbb{S}^{d-1})$ given by

$$(f, g) = \int_{|\xi|=1} f(\xi) g(\xi)\, d\omega(\xi),$$

where $d\omega(\xi)$ denotes the surface measure on the surface of the unit sphere and

$$\omega_d = \int_{|\xi|=1} d\omega(\xi) = 2\pi^{\frac{d}{2}} \Gamma\left(\frac{d}{2}\right)$$

its total area.

The space $\mathcal{H}_d^n$ of *spherical harmonics of degree n* in d variables has dimension

$$c_{n,d} = \binom{n+d-2}{n} + \binom{n+d-3}{n-1} = (2n+d-2)\frac{(n+d-3)!}{n!(d-2)!}$$

and there can be chosen an orthogonal basis $S_{n,j}$, $j = 1, \ldots, c_{n,d}$, in $\mathcal{H}_d^n$ such that

$$(S_{n,j}, S_{k,l}) = \delta_{nk}\delta_{jl}. \tag{2.11}$$

Given such an orthogonal basis the basis elements satisfy an *addition formula*

$$\sum_{j=1}^{c_{n,d}} S_{n,j}(\xi)S_{n,j}(\eta) = \frac{c_{n,d}}{\omega_d}\,\frac{C_n^{\lambda}(\xi^t\eta)}{C_n^{\lambda}(1)}. \tag{2.12}$$

Letting d tend to 2 this formula reduces to the classical addition formula for the cosine function.

The addition formula is a fundamental relation in the context of functions on the sphere, since it allows to represent *zonal functions*, i.e., functions depending on $\xi^t\eta$, $\xi, \eta \in \mathbb{S}^{d-1}$, only, in terms of Gegenbauer expansions. There is a group theoretic explanation for the connection between spherical harmonics and Gegenbauer polynomials (cf. [10] for details). We do not want to unfold the theory in the context of this paper, but let us briefly mention that from the group theory point of view Gegenbauer expansions are a natural tool to deal with zonal functions on the sphere.

To relate radial functions on $\mathbb{R}^d$ with zonal functions on $\mathbb{S}^{d-1}$, recall that the *geodesic distance* of two points on $\mathbb{S}^{d-1}$ is defined as $d(\xi, \eta) = \arccos \xi^t\eta$, $\xi, \eta \in \mathbb{S}^{d-1}$. The Euclidean distance between ξ and η then is $|\xi - \eta| = \sqrt{2 - 2\xi^t\eta}$. Thus, if ϕ is positive definite and radial on $\mathbb{R}^d$,

$$\psi(\xi, \eta) = \phi\left(\sqrt{2 - 2\xi^t\eta}\right), \qquad \xi, \eta \in \mathbb{S}^{d-1},$$

is positive definite and zonal on $\mathbb{S}^{d-1}$.

To discuss the aforementioned conjecture in detail, let us first broaden the concept of positive definite functions to enlarge the class of suitable basis functions. A radial function $\phi : \mathbb{R}^d \to \mathbb{R}$ is said to be *conditionally positive definite of order k*, if the sum (1.1) is non-negative for all finite sets of points $x_1, \ldots, x_n$ in $\mathbb{R}^d$ and all coefficients $c_1, \ldots, c_n$ satisfying

$$\sum_{j=1}^{n} c_j p(x_j) = 0$$

for all polynomials p on $\mathbb{R}^d$ of degree less than k. Clearly, positive definite functions are conditionally positive definite of order 0. Micchelli [14] gave a sufficient condition to ensure that a function is conditionally positive definite on all spaces $\mathbb{R}^d$, $d \geqslant 1$, which later has been shown to be necessary by Guo et al. [9]. For fixed $d \geqslant 1$ characterizations of conditionally positive definite functions can be found, for example, in the book of Gel'fand and Vilenkin [8, Chapter II].

To state Micchelli's condition, we need the following definition. A continuous function ϕ on $[0, \infty)$ is said to be *completely monotone* on $(0, \infty)$, if $f \in C^{\infty}(0, \infty)$ and for all $m \in \mathbb{N}_0$ we have $(-1)^m f^{(m)}(t) \geqslant 0$, for all $t \in (0, \infty)$.

Theorem B. *Let ϕ be continuous on $[0, \infty)$ and $(-1)^k \phi^{(k)}$ be completely monotone on $(0, \infty)$. Then ϕ is radial and conditionally positive definite of order k on all spaces $\mathbb{R}^d$, $d \geqslant 1$.*

Using Theorem B, we can conclude that Levesley and Hubbert obviously had conditionally positive definite functions in mind when they formulated their conjecture. We can thus alter its formulation by assuming that the function ϕ is conditionally positive definite on $\mathbb{R}^d$ for all $d \geqslant 1$. We will use a representation of conditionally positive definite functions on $\mathbb{R}^d$ for fixed dimension d. Therefore, we state the conjecture for the larger class of conditionally positive definite radial functions for fixed dimension.

The formulation of the conjecture in [12] assumes the function $\widehat{\phi}$ to have polynomial decay which usually has to be understood as a condition on the decay of the function as the argument tends to ∞. But, as we will show below, the behavior of the Fourier transform $\widehat{\phi}$ for large arguments does not influence the decay of the coefficients d_n as $n \to \infty$. At a first glance, this seems to be surprising. From the heuristic argument that smoothness of the function ϕ corresponds to decay of its Fourier transform for large arguments, one might conclude that since ϕ and ψ could in some way be identified, we should expect a certain decay of the Fourier transform of ψ, i.e., its zonal series expansion, given a smooth function ϕ.

In a certain way this argument is correct, although it is a priori not clear in what sense smoothness of the function ψ has to be understood. But due to the restriction to the sphere, ϕ and ψ coincide on the interval $[0, 1]$, only. On the other hand, any inference on the smoothness of ϕ out of its Fourier transform is of global nature, i.e., takes the whole positive real axis into account. Since we can scale the sphere by an arbitrary factor $\varepsilon > 0$, the only region where we can expect any influence of the behavior of $\widehat{\phi}$ on the decay of the coefficients d_n, is close to the origin. Thus, we have to further modify the conjecture, assuming a certain behavior of the function $\widehat{\phi}$ close to the origin.

Dealing with generalized functions and their Fourier transforms indeed allows a singularity of $\widehat{\phi}$ at the origin. Crum [4], for example, showed that the Fourier transform of a measurable positive definite radial function is continuous on $(0, \infty)$ and can at most have a singularity at the end points.

Summarizing the above arguments, we end up with the following clarified version of the conjecture:

Conjecture C. *Let ϕ be conditionally positive definite of order k, $k \in \mathbb{N}_0$, and radial on $\mathbb{R}^d$. Assume further that the generalized Fourier transform of ϕ exists and satisfies*

$$\widehat{\phi}(t) = \mathcal{O}(t^{-2k-\gamma}), \qquad \text{as } t \to 0$$

for some $\gamma > 0$. If

$$\psi(\xi, \eta) = \sum_{n=0}^{\infty} d_n \sum_{k=1}^{c_{n,d}} S_{n,k}(\xi) S_{n,k}(\eta), \qquad \xi, \eta \in \mathbb{S}^{d-1},$$

denotes the zonal series expansion of the restriction of ϕ to the sphere, i.e.,

$$\psi(\xi, \eta) = \phi\left(\sqrt{2 - 2\,\xi^t \eta}\right), \qquad \xi, \eta \in \mathbb{S}^{d-1},$$

then the Fourier coefficients $\{d_n\}_{n\in\mathbb{N}_0}$ *have an analog decay rate. To be precise,*

$$d_n = \mathcal{O}\left(n^{-2k-\gamma+1}\right), \qquad \text{as } n \to \infty.$$

We will prove the case $k = 0$ first, i.e., for positive definite functions ϕ. The general case then follows in Section 4.

3. Gegenbauer expansion of a radial function

Since for $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, $a = |\mathbf{x}|$, $b = |\mathbf{y}|$, and $c = |\mathbf{x} - \mathbf{y}|$ form a triangle we can use the addition theorem (2.9) to obtain a Gegenbauer expansion for the kernel of the inverse Fourier–Bessel transform.

Let ϕ be a function on $\mathbb{R}_+$ such that its inverse Fourier–Bessel transform exists. Following (2.3) we can write

$$\begin{aligned}\phi(c) &= c^{-\lambda} \int_0^\infty J_\lambda(ct)\widehat{\phi}(t)t^{\lambda+1}\,dt\\ &= 2^\lambda \Gamma(\lambda) \sum_{n=0}^\infty \left(\lambda+n\right) C_n^\lambda\left(\frac{\mathbf{x}^t\mathbf{y}}{ab}\right) \int_0^\infty \frac{J_{\lambda+n}(at)}{(at)^\lambda}\,\frac{J_{\lambda+n}(bt)}{(bt)^\lambda}\,\widehat{\phi}(t)t^{2\lambda+1}\,dt.\end{aligned}$$

Denoting the integral

$$I_{d,n}^{(a,b)}(\widehat{\phi}) = \int_0^\infty \frac{J_{\lambda+n}(at)}{(at)^\lambda}\,\frac{J_{\lambda+n}(bt)}{(bt)^\lambda}\,\widehat{\phi}(t)t^{2\lambda+1}\,dt$$

and $I_{d,n}(\widehat{\phi}) = I_{d,n}^{(1,1)}(\widehat{\phi})$, we finally have

$$\phi(c) = 2^\lambda \Gamma(\lambda) \sum_{n=0}^\infty (\lambda+n) I_{d,n}^{(a,b)}(\widehat{\phi}) C_n^\lambda(\cos\,\theta), \tag{3.1}$$

where $ab\cos\theta = \mathbf{x}^t\mathbf{y}$ for $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$.

If $|\mathbf{x}| = |\mathbf{y}| = 1$ we have $|\mathbf{x} - \mathbf{y}| = \sqrt{2 - 2\,\cos\,\theta}$. Restricting the function $\Psi(\mathbf{x}, \mathbf{y}) = \phi(|\mathbf{x} - \mathbf{y}|)$ to $\mathbb{S}^{d-1} \times \mathbb{S}^{d-1}$ we, therefore, have a zonal function $\psi(\xi, \eta) = \phi(\sqrt{2 - 2\xi^t\eta})$, for $\xi, \eta \in \mathbb{S}^{d-1}$. According to (1.2) and (2.12) we obtain

$$\begin{aligned}\psi(\xi,\eta) &= \sum_{n=0}^\infty d_n \sum_{k=1}^{c_{n,k}} S_{n,k}(\xi)S_{n,k}(\eta)\\ &= \sum_{n=0}^\infty \frac{d_n c_{n,d}}{\omega_d}\,\frac{C_n^\lambda(\cos\,\theta)}{C_n^\lambda(1)} = \frac{\Gamma(\lambda)}{2\pi^{\lambda+1}} \sum_{n=0}^\infty (n+\lambda) d_n C_n^\lambda(\cos\,\theta).\end{aligned} \tag{3.2}$$

Since $\phi(c) = \psi(\xi, \eta)$, comparing coefficients in (3.1) and (3.2) gives

$$d_n = (2\pi)^{\lambda+1} I_{d,n}(\widehat{\phi}), \qquad n \in \mathbb{N}_0. \tag{3.3}$$

We, therefore, have proved the following relation between the coefficients d_n of the zonal series expansion of ψ and the integrals $I_{d,n}(\widehat{\phi})$.

Proposition 1. *Let $\phi : \mathbb{R}_+ \to \mathbb{R}$ be a function such that its inverse Fourier–Bessel transform exists, and $\lambda = \frac{d-2}{2}$. Further assume the integrals*

$$I_{d,n}(\widehat{\phi}) \;=\; \int_0^\infty J^2_{\lambda+n}(t)\,\widehat{\phi}(t)\,t\,dt \tag{3.4}$$

exist for all $n \in \mathbb{N}_0$, where $\widehat{\phi}$ denotes the Fourier–Bessel transform (2.3) *of ϕ. Let ψ be the zonal function defined by*

$$\psi\left(\xi,\eta\right) \;=\; \phi(\sqrt{2-2\xi^t\eta}), \qquad \xi,\eta \in \mathbb{S}^{d-1}.$$

Then the coefficients d_n in the series expansion (1.2) *of ψ are given by*

$$d_n \;=\; (2\pi)^{\lambda+1}\, I_{d,n}(\widehat{\phi}), \qquad n \in \mathbb{N}_0. \tag{3.5}$$

Proposition 1 appeared in a similar form in [16, Theorem 4.1] but the proof given there does not use Gegenbauer's addition theorem (2.9). However, the appearance of the addition theorem has a deeper structural reason coming from the relation between the two geometric settings involved here. The latter are closely related to the Bessel functions and the Gegenbauer polynomials, respectively. We cannot go into the details of this connection, here. The interested reader is referred to [10, Chapter IV] and especially to the work by Flensted-Jensen and Koornwinder [6].

To analyze the behavior of $I_{d,n}(\widehat{\phi})$ with respect to n we choose $\tau > 0$ and decompose the integral

$$I_{d,n}(\widehat{\phi}) \;=\; \int_0^\tau J^2_{\lambda+n}(t)\widehat{\phi}(t)t\,dt \;+\; \int_\tau^\infty J^2_{\lambda+n}(t)\widehat{\phi}(t)t\,dt. \tag{3.6}$$

From the asymptotic expansion of the Bessel functions (cf. [1, (4.8.5)])

$$J_\nu(t) \;\sim\; \sqrt{\frac{2}{\pi t}}\cos\left(t-\frac{\nu\pi}{2}-\frac{\pi}{4}\right)+\mathcal{O}\left(\frac{1}{t}\right) \tag{3.7}$$

for large t, the second integral reads, with $\tau > 0$ sufficiently large,

$$\int_\tau^\infty J^2_{\lambda+n}(t)\widehat{\phi}(t)t\,dt \sim \frac{2}{\pi}\int_\tau^\infty \widehat{\phi}(t)\cos^2\left(t-\frac{(n+\lambda)\pi}{2}-\frac{\pi}{4}\right)dt+\mathcal{O}\left(\frac{1}{\tau}\right). \tag{3.8}$$

Setting $\alpha = t-\frac{\lambda}{2}\pi-\frac{\pi}{4}$, consider the product

$$\cos\left(\alpha-\frac{\pi}{2}n\right)\cos\left(\alpha-\frac{\pi}{2}n\right).$$

If n is even, $\cos\left(\alpha-\frac{\pi}{2}n\right) = \pm\cos\alpha$, and if n is odd, $\cos\left(\alpha-\frac{\pi}{2}n\right) = \mp\sin\alpha$. Therefore, the integrand in (3.8) is independent of n, assuming $\widehat{\phi}$ is such that the integral exists.

It remains to find an asymptotic expansion in n for the first integral in (3.6). Since the decay of coefficients (3.3) for large n is dominated by the behavior of integral (3.4) close to the origin, we can use the assumption on the behavior of the Fourier transform of ϕ as given in Conjecture C, for $k=0$, to estimate the integral.

From [1, Ex.4.15] we have for $2\nu+1>\beta>-1$

$$\int_0^\infty x^{-\beta} J_\nu^2(x)\,dx \;=\; \frac{\Gamma(\beta)\Gamma\left(\nu+\frac{1-\beta}{2}\right)}{2^\beta \Gamma^2\left(\frac{\beta+1}{2}\right)\Gamma\left(\nu+\frac{\beta+1}{2}\right)}.$$

This is a special case of Gauss' summation formula for a hypergeometric ${}_2F_1$-series applied to an integral of Sonine–Schaftheitlin (cf. [1, Chapter 4] for details).

Using $\frac{\Gamma(\nu+\kappa)}{\Gamma(\nu+\rho)} = \mathcal{O}(\nu^{\kappa-\rho})$ for $\nu\to\infty$, we have

$$\int_0^\infty x^{-\beta} J_\nu^2(x)\,dx \;=\; \frac{\Gamma(\beta)\Gamma\left(\nu+\frac{1-\beta}{2}\right)}{2^\beta \Gamma^2\left(\frac{\beta+1}{2}\right)\Gamma\left(\nu+\frac{\beta+1}{2}\right)} \;=\; \mathcal{O}(\nu^{-\beta}) \tag{3.9}$$

for large ν, provided $2\nu+1>\beta>-1$.

Since the second integral in (3.6) is independent of n, and we are interested in the asymptotic behavior of the coefficients d_n for large n, only, we can replace the function $\widehat{\phi}(t)$ in the integral (3.4) by $t^{-\gamma}$ assuming that $\widehat{\phi}(t)=\mathcal{O}(t^{-\gamma})$ for $t\to 0$. But we have to make sure that the integral (3.4) exists. From the asymptotic behavior of the Bessel functions (3.7) and the series representation (2.2), respectively, we have

$$J_\nu(t)=\mathcal{O}(t^\nu), \quad \text{as } t\to 0,$$
$$J_\nu(t)=\mathcal{O}\left(t^{-\frac{1}{2}}\right), \quad \text{as } t\to\infty.$$

Therefore, the integral exists if $2\nu+1>\beta>-1$. Setting $\beta=\gamma-1$ and $\nu=\lambda+n$ the condition reads $d+2n>\gamma>0$. This inequality has to be satisfied for all $n\in\mathbb{N}$, therefore, $d>\gamma>0$. We thus proved the following result:

Theorem 2. *If the generalized Fourier–Bessel transform $\widehat{\phi}$ of a positive definite radial function ϕ exists, and for some $0<\gamma<d$*

$$\widehat{\phi}(t) \;=\; \mathcal{O}(t^{-\gamma}), \qquad \text{as } t\to 0,$$

then the coefficients d_n in the zonal series expansion

$$\psi(\xi,\eta) \;=\; \phi(\sqrt{2-2\xi^t\eta}) \;=\; \sum_{n=0}^\infty d_n \sum_{k=1}^{c_{n,k}} S_{n,k}(\xi)S_{n,k}(\eta), \qquad \xi,\eta\in\mathbb{S}^{d-1},$$

satisfy

$$d_n \;=\; \mathcal{O}(n^{-\gamma+1}), \qquad \text{as } n\to\infty.$$

The condition $\gamma<d$ in Theorem 2 does not really mean a restriction. From the asymptotic behavior of the Bessel function close to zero and the existence of the integral (2.3) we

conclude that $\widehat{\phi}(t)$ cannot grow faster than $t^{2\lambda+2} = t^d$ as $t \to 0$. Therefore, the upper bound $\gamma < d$ is naturally given by the existence of the Fourier–Bessel transform.

4. Conditionally positive definite functions

We now want to extend the result in Theorem 2 to conditionally positive definite functions. Again, let $\phi \in L^1_{\text{loc}}(\mathbb{R}^d)$ be a function of polynomial growth. ϕ is a conditionally positive definite generalized function of order k on $\mathcal{S}(\mathbb{R}^d)$ if it can be represented as (cf. [8, II 4.4(25)])

$$\int_{\mathbb{R}} \phi(\mathbf{x})\varphi(\mathbf{x})\,d\mathbf{x} = \int_{\mathbb{R}_0\setminus\{0\}} \left[\widehat{\varphi}(\mathbf{v}) - \alpha(\mathbf{v}) \sum_{|n|=0}^{2k-1} \frac{\widehat{\varphi}^{(n)}(0)}{n!}\mathbf{v}^k\right] d\mu(\mathbf{v}) + \sum_{|n|=0}^{2k} \frac{\widehat{\varphi}^{(n)}(0)}{n!} a_n, \tag{4.1}$$

where μ is a positive tempered measure such that $\int_{0<|\mathbf{v}|<1} |\mathbf{v}|^{2k}\,d\mu(\mathbf{v}) < \infty$. The function $\alpha \in \mathcal{S}(\mathbb{R}^d)$ has to be chosen such that $\alpha(\cdot) - 1$ has a zero of order $2k+1$ at the origin, and a_k are certain coefficients depending on ϕ and α (for further details, see [8]). Applying the Fourier–Bessel transform for conditionally positive definite radial functions of order k to this representation, we derive the expression

$$\phi(\rho) = k_\lambda \int_0^\infty \left(\mathcal{J}_\lambda(\rho t) - \alpha(t) \sum_{l=0}^{k-1} \frac{(-1)^l(\rho t)^{2l}}{4^l\Gamma(\lambda+l+1)}\right) t^{2\lambda+1}\,d\mu(t) + \sum_{l=0}^{k-1} \frac{(-1)^l}{4^l\Gamma(\lambda+l+1)}\, a_l \rho^{2l}. \tag{4.2}$$

The measure μ now denotes a positive tempered measure on $\mathbb{R}_+$ satisfying

$$\int_0^1 t^{2k}\,d\mu(t) < \infty. \tag{4.3}$$

Similar representations for conditionally positive definite functions have been given in [13,9]. For our purposes it is not necessary to specify the function α and the coefficients a_k explicitly.

To proceed in the same way as for the case $k = 0$ we need the expansion of the kernel of this representation in terms of Gegenbauer polynomials. Observe, that the second term of sum (4.2) is a polynomial of degree less or equal $2k - 2$. Since we are interested in the behavior of the coefficients d_n for large n, we can, without loss of generality, alter the function ϕ by adding a polynomial to make this term disappear. For the integral term we use a similar argumentation. The function

$$\mathcal{J}_\lambda(\rho t) - \alpha(t) \sum_{l=0}^{k-1} \frac{(-1)^l(\rho t)^{2l}}{4^l\Gamma(\lambda+l+1)}, \quad \rho, t \in \mathbb{R}_+, \tag{4.4}$$

differs from $\mathcal{J}_\lambda$ by a polynomial of degree at most $2k-2$ as function of ρ. Since the coefficients in the Gegenbauer expansion of a function are unique and the space of polynomials decomposes into a direct sum of spaces of polynomials of fixed degree, the Gegenbauer coefficients of the function (4.4) equal

$$4^\lambda \Gamma(\lambda)\Gamma(\lambda+1)(\lambda+n)\,\frac{J_{\lambda+n}(at)}{(at)^\lambda}\,\frac{J_{\lambda+n}(bt)}{(bt)^\lambda}$$

for $n \geqslant k$, where a, b and ρ are the lengths of the sides of a triangle. Again, we ignore the lower order coefficients. We can, therefore, use the same expansion as in the case $k = 0$. Thus, we have to analyze the integral

$$I_{d,n}(\widehat{\phi}) = \int_0^\infty J^2_{\lambda+n}(t)\widehat{\phi}(t)\,t\,dt \qquad \text{for } n \geqslant k. \tag{4.5}$$

We can again use (3.9) to estimate the behavior of the coefficients d_n for large n.

Theorem 3. *If for some $0 < \gamma < d$ the generalized Fourier transform of a radial function ϕ which is conditionally positive definite of order $k \in \mathbb{N}_0$ satisfies*

$$\widehat{\phi}(t) = \mathcal{O}(t^{-2k-\gamma}), \qquad \text{as } t \to 0,$$

then the coefficients d_n in the zonal series expansion

$$\psi(\xi,\eta) = \phi(\sqrt{2-2\xi^t\eta}) = \sum_{n=0}^\infty d_n \sum_{k=1}^{c_{n,k}} S_{n,k}(\xi)S_{n,k}(\eta), \qquad \xi,\eta \in \mathbb{S}^{d-1},$$

satisfy

$$d_n = \mathcal{O}(n^{-2k-\gamma+1}), \qquad \text{as } n \to \infty.$$

From condition (4.3) on the measure μ we can conclude that $d\mu(t) = \widehat{\phi}(t)\,dt$ can have a singularity of order $2k$ at the origin. This fact is implicitly stated in the assumption on $\widehat{\phi}$. The condition for estimate (3.9) now reads $2\lambda + 2n + 1 > 2k + \gamma + 1 > -1$. Since $n \geqslant k$, the inequalities are satisfied for $0 < \gamma < d$. Again, the upper bound does not really mean a severe restriction.

5. Remarks and open questions

To motivate the discussion concerning a possible relation between the function $\widehat{\phi}$ and the Gegenbauer coefficients d_n based on smoothness of the function ϕ, let us briefly sketch the background. Starting with a generalized function Φ on $\mathbb{R}$, we can define its Fourier transform $\widehat{\Phi}$ in the usual way. Assuming that for some $\kappa \in \mathbb{N}$, the inverse Fourier transform of the function $\widehat{\Phi^{(\kappa)}}$ exists, it is well-known that

$$\widehat{\Phi^{(\kappa)}}(\mathbf{v}) = (i\mathbf{v})^\kappa \widehat{\Phi}(\mathbf{v}), \qquad \mathbf{v} \in \mathbb{R}. \tag{5.1}$$

Putting this relation into a proper context, gives an interpretation of smoothness of Φ derived from its Fourier transform.

Let us now analyze this relation for the case where $\Phi : \mathbb{R}^d \to \mathbb{R}$ has certain symmetries. The group GL_d of invertible $d \times d$ matrices acts on $\mathbb{R}^d$ via linear transformations. Likewise, it naturally acts on functions on $\mathbb{R}^d$ by setting $f \circ A(\mathbf{x}) = f(A\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^d$, $A \in GL_d$. Using this concept, symmetry can be interpreted as invariance with respect to the action of a subgroup $K \leqslant GL_d$, i.e., $f(A\mathbf{x}) = f(\mathbf{x})$ for all $A \in K$. For example, if Φ is radial, then

$$\Phi(A\mathbf{x}) = \Phi(\mathbf{x}) \qquad \text{for all } A \in SO_d.$$

We can then identify the function Φ with a function ϕ which is defined on the set of equivalence classes, i.e., the orbit space $(\mathbb{R}^d)^K$ of the group action. $(\mathbb{R}^d)^K$ can be identified with a certain subset of $\mathbb{R}^d$ and Φ with a function ϕ on $(\mathbb{R}^d)^K$. In the above example, $(\mathbb{R}^d)^{SO_d} = \mathbb{R}_+$ and Φ is identified with ϕ by means of $\Phi(\mathbf{x}) = \phi(|\mathbf{x}|)$, $\mathbf{x} \in \mathbb{R}^d$. With this relation in mind, we can ask for relations between differentiability properties of the functions Φ and ϕ.

For radial functions there is a one-to-one correspondence. By a theorem of Ball [2], $\Phi \in C^\kappa(\mathbb{R}^d)$ if and only if $\phi \in C^\kappa(\mathbb{R})$, where $\kappa \geqslant 0$, and ϕ is extended to an even function on $\mathbb{R}$. Therefore, the notion of smoothness on $\mathbb{R}^d$ induced by the classical derivative carries over to smoothness on $\mathbb{R}$, using the classical derivative on $\mathbb{R}$, and the Fourier transform reflects these connections. Since Ball assumes continuity over all of $\mathbb{R}^d$ generalized Fourier transforms are ruled out. Passing to generalized Fourier transforms for radial functions, we can allow a singularity at the origin (cf. [4]). As shown by the above analysis, this singularity determines the behavior of the Gegenbauer coefficients.

The same question turns out to be more complicated for zonal functions on the sphere. First, we have to identify a zonal function ψ on $\mathbb{S}^{d-1}$ as the restriction of an invariant function on $\mathbb{R}^d$ onto the orbit space of a group action. Let Λ_d^+ be the subgroup of GL_d spanned by rotations which fix one of the coordinate axes, the dth, say, and by non-negative multiples of the identity matrix. Note that both types of generators can be identified with a subgroup of GL_d. If a function Φ on $\mathbb{R}^d$ is invariant under scaling the components of its argument, it is uniquely defined by the values on a sphere of arbitrary radius. Assuming further that Φ is invariant under rotations around the d-axis, Φ can be identified with a zonal function ψ on the sphere. On the other hand, every zonal function on the sphere can be extended to a function Φ on $\mathbb{R}^d$ defining $\Phi(\mathbf{x}) = \psi(\mathbf{x}/|\mathbf{x}|, \mathbf{e}_1)$ for all $\mathbf{x} \in \mathbb{R}^d$, where $\mathbf{e}_1$ denotes the first standard unit vector in $\mathbb{R}^d$.

The question of differentiability is much more involved here. We are not aware of a result comparable to the one by Ball for this setting. Nevertheless, there are relations between the Gegenbauer coefficients of ψ and the coefficients of its derivatives.

Assume that $\psi(\xi, \eta)$ is a zonal function on $\mathbb{S}^{d-1}$ with zonal series expansion

$$\psi(t) = \sum_{n=0}^{\infty} d_n C_n^\lambda(t), \qquad t = \cos(\xi^t \eta), \quad \xi, \eta \in \mathbb{S}^{d-1}.$$

Assume further, that ψ is κ-times differentiable considered as an even function on $[-1, 1]$, and let $d_n^{(\kappa)}$ denote the Gegenbauer coefficients of the zonal series representation of $\psi^{(\kappa)}$.

The relation between the coefficients d_n and $d_n^{(\kappa)}$ has been studied by several authors. In [5] for instance, one finds

$$d_n^{(\kappa)} = \frac{2^\kappa (n+\lambda)\Gamma(n+2\lambda)}{\Gamma(\kappa)\Gamma(n+1)} \times \sum_{j=1}^{\infty} (j)_{\kappa-1} \frac{\Gamma(n+j+\kappa+\lambda-1)\Gamma(n+2j+\kappa-1)}{\Gamma(n+j+\lambda)\Gamma(n+2j+\kappa+2\lambda-2)} d_{n+2j+\kappa-2}.$$

From this one can obtain the rather crude estimate

$$d_n^{(\kappa)} = \mathcal{O}(n^{\kappa+\beta}), \qquad \text{as } n \to \infty,$$

assuming that $d_n = \mathcal{O}(n^\beta)$, as n tends to infinity. Thus, smoothness of even extension of the function on $[-1, 1]$ corresponds to a certain decay of the Fourier coefficients as n tends to infinity.

It is a challenging problem to give a full explanation for the relation in Theorems 2 and 3. There are two questions which are linked together. First, what is the correct interpretation of smoothness for functions on $\mathbb{R}_+$ and $\mathbb{S}^{d-1}$, respectively, such that the heuristic argument of smoothness corresponds to decay of the Fourier transform, can be put into a rigorous framework. Second, how do the assumingly different concepts of smoothness link together using the common interpretation that the functions under consideration are restrictions of K-invariant functions on $\mathbb{R}^d$ to the orbit space $(\mathbb{R}^d)^K$.

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