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CONVOLUTION ROOTS AND DIFFERENTIABILITY OF ISOTROPIC POSITIVE DEFINITE FUNCTIONS ON SPHERES

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ABSTRACT. We prove that any isotropic positive definite function on the sphere can be written as the spherical self-convolution of an isotropic real-valued function. It is known that isotropic positive definite functions on d-dimensional Euclidean space admit a continuous derivative of order $[(d-1)/2]$. We show that the same holds true for isotropic positive definite functions on spheres and prove that this result is optimal for all odd dimensions.

1. INTRODUCTION

For an integer $d \in \mathbb{N}$ we denote the d-dimensional unit sphere by $\mathbb{S}^d = \{x \in \mathbb{R}^{d+1} \mid \|x\| = 1\}$, where $\|\cdot\|$ denotes the Euclidean norm on $\mathbb{R}^{d+1}$. A function $f : \mathbb{S}^d \times \mathbb{S}^d \to \mathbb{R}$ is *positive definite* if

$$\sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j f(u_i, u_j) \geq 0 \tag{1.1}$$

for all $u_1, \dots, u_n \in \mathbb{S}^d$ and coefficients $c_1, \dots, c_n \in \mathbb{R}$. The function f is *isotropic* if there exists a function $\bar{f} : [0, \pi] \to \mathbb{R}$ that fulfills

$$f(u, v) = \bar{f}(\theta(u, v)) \quad \text{for all } u, v \in \mathbb{S}^d, \tag{1.2}$$

where the geodesic distance on $\mathbb{S}^d$ is given by $\theta : \mathbb{S}^d \times \mathbb{S}^d \to \mathbb{R}$, $\theta(u, v) = \arccos(\langle u, v\rangle)$. Here, $\langle \cdot, \cdot \rangle$ denotes the standard scalar product on $\mathbb{R}^{d+1}$.

Isotropic positive definite functions on spheres occur in statistics as correlation functions of homogeneous random fields on spheres or of star-shaped random particles. They also have applications in approximation theory where they are used as radial basis functions for interpolating scattered data on spherical domains. Recent applications in spatial statistics can be found in [1, 12, 13]; application examples in approximation theory are given in [4, 9, 26].

The class Ψ_d consists of all continuous functions $\psi : [0, \pi] \to \mathbb{R}$ with $\psi(0) = 1$, such that the isotropic function $\psi(\theta(\cdot, \cdot))$ is positive definite. The classes Ψ_d are nonincreasing in d,

$$\Psi_1 \supset \Psi_2 \supset \cdots \supset \Psi_\infty = \bigcap_{d=1}^{\infty} \Psi_d,$$

with the inclusions being strict; see [11, Corollary 1].

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We define the *spherical convolution* of two isotropic functions $f, g : \mathbb{S}^d \times \mathbb{S}^d \to \mathbb{R}$ as

$$(f \circledast g)(u, v) = \int_{\mathbb{S}^d} \bar{f}(\theta(u, w))\bar{g}(\theta(w, v))dw, \quad \text{for all } u, v \in \mathbb{S}^d,$$

where the integration is with respect to the d-dimensional Hausdorff measure on $\mathbb{S}^d$. The total measure of $\mathbb{S}^d$ is denoted by $\sigma_d = 2\pi^{(d+1)/2}/\Gamma((d+1)/2)$. It is easy to see that the spherical self-convolution of any isotropic L^2-function f on $\mathbb{S}^d \times \mathbb{S}^d$ is positive definite. A function $\varphi : [0, \pi] \to \mathbb{R}$ has a *spherical convolution root* if there exists an isotropic function $g : \mathbb{S}^d \times \mathbb{S}^d \to \mathbb{R}$ such that $\varphi(\theta(\cdot, \cdot)) = g \circledast g$.

Spherical convolution has been used by several authors [8, 12, 21, 25] as a tool to construct spherical positive definite functions. It is natural to ask the reverse question: Which functions can be obtained through this construction principle? We can give the following general positive answer, which we prove in Section 3.

Theorem 1.1. *Any $\psi \in \Psi_d$ has a spherical convolution root which can be taken to be real-valued and isotropic.*

The techniques used to show the convolution representation theorem have led to the solution of a further interesting problem concerning positive definite functions on spheres.

A positive definite function f on $\mathbb{R}^d$ is defined analogously to (1.1). The function f is called radial if $f(x, y) = \tilde{f}(\|x - y\|)$ for some function $\tilde{f} : [0, \infty) \to \mathbb{R}$. Schoenberg [19, Lemma 4] showed that radial positive definite functions on $\mathbb{R}^d$ have a continuous derivative of order $[(d-1)/2]$, where $[c]$ denotes the greatest integer less than or equal to c. The following theorem, which will be shown in Section 4.1 confirms the conjecture of Gneiting [11] that the same holds true on spheres.

Theorem 1.2. *The functions in the class Ψ_d admit a continuous derivative of order $[(d-1)/2]$ on the open interval $(0, \pi)$.*

The derivatives at the point $\vartheta = 0$ can be infinite or can take finite values. We believe that the same holds true at $\vartheta = \pi$. However, we are currently not able to provide simple examples for the latter claim. The *powered exponential family*

$$\psi(\vartheta) = \exp\Big(-\Big(\frac{\vartheta}{c}\Big)^{\alpha}\Big), \quad \vartheta \in [0, \pi],$$

with parameters $c > 0$ and $\alpha \in (0, 1]$ belongs to Ψ_∞ [11]. For $\alpha < 1$ the first derivative at zero is $-\infty$, whereas for $\alpha = 1$ it takes the value $-1/c$. The *sine power function*

$$\psi(\vartheta) = 1 - \Big(\sin\frac{\vartheta}{2}\Big)^{\alpha}, \quad \vartheta \in [0, \pi],$$

as in [22] is a member of Ψ_∞ for $\alpha \in [0, 2]$. For $\alpha \in (0, 1)$, the first derivative at zero is $-\infty$; for $\alpha = 1$, we obtain $\psi'(0) = -1/2$. If $\alpha \in (1, 2]$, the derivative at zero is zero.

In the Euclidean case it is known that Theorem 1.2 is the best possible [10]. Hence, there are radial positive definite functions on $\mathbb{R}^d$ whose derivative of order $[(d-1)/2] + 1$ is not continuous. The optimality of Theorem 1.2 for $d = 1, 3, 5, 7$ follows from the results in [2]. In Section 4.2 we introduce a turning bands operator for isotropic positive definite functions on spheres to show the optimality of Theorem 1.2 for all odd dimensions. In even dimensions it remains an open problem. However, once the optimality can be shown for $d = 2$, the turning bands operator immediately yields the assertion in all even dimensions as well.

The convolution representation result, Theorem 1.1, also has consequences that are of interest in statistical applications. Firstly, it shows that any isotropic covariance function on the sphere can be obtained by the Lévy based approach to modelling star-shaped random particles introduced in [12]. Secondly, the proof of Theorem 1.1 reveals a way to resolve the identifiability issues associated with these models. It is possible to distinguish one specific convolution root amongst all possible convolution roots of a given covariance function. This is the basis of the inference procedure described in [27].

2. Convolution of isotropic functions on spheres

Let $L^2(\mathbb{S}^d \times \mathbb{S}^d)$ be the space of square-integrable functions on $\mathbb{S}^d \times \mathbb{S}^d$ with the Hausdorff measure. By $\langle \cdot, \cdot \rangle_{L^2}$ and $\|\cdot\|_{L^2}$ we denote the scalar product and the norm of the Hilbert space $L^2(\mathbb{S}^d \times \mathbb{S}^d)$, respectively. We consider the subspace $L^2_{d,\mathcal{I}} \subset L^2(\mathbb{S}^d \times \mathbb{S}^d)$ of functions that are isotropic as defined at (1.2). For $f \in L^2_{d,\mathcal{I}}$ it holds for all $d+1$-dimensional orthogonal matrices R that

$$f(Ru, Rv) = \bar{f}(\theta(Ru, Rv)) = \bar{f}(\theta(u, v)) = f(u, v), \quad u, v \in \mathbb{S}^d.$$

This property characterizes the functions in $L^2_{d,\mathcal{I}}$.

Proposition 2.1. *The convolution $f \circledast g$ of $f, g \in L^2_{d,\mathcal{I}}$ is in $L^2_{d,\mathcal{I}}$ and*

$$\|f \circledast g\|_{L^2} \leq \sigma_d \sup_{u,v \in \mathbb{S}^d} |(f \circledast g)(u, v)| \leq \|f\|_{L^2} \|g\|_{L^2}. \tag{2.1}$$

The convolution is bilinear, commutative and

$$\|f \circledast g\|^2_{L^2} = \langle f \circledast f, g \circledast g \rangle_{L^2}. \tag{2.2}$$

Proof. It is easy to check that $f \circledast g$ is isotropic. Furthermore, by Hölder's inequality,

$$\begin{aligned}
|(f \circledast g)(u, v)| &\leq \int_{\mathbb{S}^d} |\bar{f}(\theta(u, w)) \bar{g}(\theta(w, v))| dw \\
&\leq \left\{ \int_{\mathbb{S}^d} \bar{f}(\theta(u, w))^2 dw \right\}^{\frac{1}{2}} \left\{ \int_{\mathbb{S}^d} \bar{g}(\theta(w, v))^2 dw \right\}^{\frac{1}{2}} \\
&\overset{(*)}{=} \left\{ \frac{1}{\sigma_d} \int_{\mathbb{S}^d \times \mathbb{S}^d} \bar{f}(\theta(u, w))^2 dw du \right\}^{\frac{1}{2}} \left\{ \frac{1}{\sigma_d} \int_{\mathbb{S}^d \times \mathbb{S}^d} \bar{g}(\theta(w, v))^2 dw dv \right\}^{\frac{1}{2}} \\
&= \frac{1}{\sigma_d} \|f\|_{L^2} \|g\|_{L^2}
\end{aligned}$$

for $u, v \in \mathbb{S}^d$. The equality at $(*)$ holds true because the integrals on the left hand side do not depend on u, v, respectively. Therefore, we obtain (2.1), and, in particular, $f \circledast g \in L^2(\mathbb{S}^d \times \mathbb{S}^d)$. Bilinearity and commutativity are clear, and equation (2.2) is an application of Fubini's theorem. □

Schoenberg [20] characterized the functions of the classes Ψ_d using Gegenbauer (or ultraspherical) polynomials. Let $\lambda > 0$. The Gegenbauer polynomials C_n^λ for $n \in \mathbb{N}_0$ are defined by the expansion

$$\frac{1}{(1 + r^2 - 2r \cos \vartheta)^\lambda} = \sum_{n=0}^{\infty} r^n C_n^\lambda(\cos \vartheta), \quad \text{for } \vartheta \in [0, \pi];$$

see [6, 18.12.4]. Note that we use $\mathbb{N}$ to denote the positive integers and $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. We will repeatedly use the fact that

$$C_n^\lambda(1) = \frac{\Gamma(n+2\lambda)}{n!\Gamma(2\lambda)}. \tag{2.3}$$

If $\lambda = 0$ we set $C_n^0(\cos\vartheta) = \cos(n\vartheta)$ for $\vartheta \in [0,\pi]$ as in [20]. We need the following important property of the Gegenbauer polynomials with $\lambda = (d-1)/2$; see for example [18, Corollary 4.9]. For $d \geq 2$, $k, n \in \mathbb{N}_0$ and $u, v \in \mathbb{S}^d$, we have

$$\int_{\mathbb{S}^d} C_k^{(d-1)/2}(\langle u,w\rangle) C_n^{(d-1)/2}(\langle w,v\rangle)dw = \delta_{k,n}\sigma_d \frac{d-1}{2n+d-1} C_n^{(d-1)/2}(\langle u,v\rangle), \tag{2.4}$$

where $\delta_{k,n}$ denotes the Kronecker delta. If $\lambda = 0$ it holds that

$$\int_{\mathbb{S}^1} C_k^0(\langle u,w\rangle) C_n^0(\langle w,v\rangle)dw = \delta_{k,n}\pi C_n^0(\langle u,v\rangle)$$

for $n \in \mathbb{N}_0$, $k \in \mathbb{N}$, $u, v \in \mathbb{S}^d$, and $\int_{\mathbb{S}^1} C_0^0(\langle u,w\rangle)C_0^0(\langle w,v\rangle)dw = 2\pi$.

Proposition 2.2. *Let $d \geq 2$. The family $\mathcal{C}_d = \{E_{d,n}\}_{n\in\mathbb{N}_0}$, where $E_{d,n} := c_{d,n}C_n^{(d-1)/2}(\langle\cdot,\cdot\rangle) \in L^2_{d,\mathcal{I}}$ with*

$$c_{d,n} = \sigma_d^{-1}\sqrt{\frac{2n+d-1}{(d-1)C_n^{(d-1)/2}(1)}},$$

is an orthonormal basis of $L^2_{d,\mathcal{I}}$. Furthermore, for $k, n \in \mathbb{N}_0$,

$$E_{d,k} \circledast E_{d,n} = \delta_{k,n}\bar{c}_{d,n}E_{d,n},$$

where

$$\bar{c}_{d,n} = \sqrt{\frac{d-1}{(2n+d-1)C_n^{(d-1)/2}(1)}}.$$

Proof. By (2.4)

$$\begin{aligned}\int_{\mathbb{S}^d\times\mathbb{S}^d} C_k^{(d-1)/2}(\langle u,v\rangle)C_n^{(d-1)/2}(\langle u,v\rangle)dudv \\ &= \delta_{k,n}\sigma_d\frac{d-1}{2n+d-1}\int_{\mathbb{S}^d} C_n^{(d-1)/2}(\langle v,v\rangle)dv \\ &= \delta_{k,n}\sigma_d^2\frac{d-1}{2n+d-1}C_n^{(d-1)/2}(1);\end{aligned}$$

hence $\mathcal{C}_d$ is an orthonormal system. It is also a Hilbert space basis, because polynomials are dense in $L^2([-1,1])$. The second assertion is a direct consequence of (2.4). □

The following proposition complements Proposition 2.2 and is not hard to prove.

Proposition 2.3. *Proposition 2.2 also holds for $d = 1$ with*

$$c_{1,n} = \begin{cases} 1/(2\pi), & \text{for } n = 0, \\ \sqrt{2}/(2\pi), & \text{for } n \geq 1, \end{cases}, \quad \bar{c}_{1,n} = \begin{cases} 1, & \text{for } n = 0, \\ \sqrt{2}/2, & \text{for } n \geq 1. \end{cases}$$

Propositions 2.2 and 2.3 imply that, for any function $f \in L^2_{d,\mathcal{I}}$, we have

$$f \overset{L^2}{=} \sum_{n\in\mathbb{N}_0} \langle f, E_{d,n}\rangle_{L^2} E_{d,n},$$

where $\overset{L^2}{=}$ means that the series on the right hand side converges unconditionally in L^2 to the left hand side. We call the basis $\mathcal{C}_d$ the *Gegenbauer basis* of $L^2_{d,\mathcal{I}}$. The coefficients $\langle f, E_{d,n}\rangle_{L^2}$ are termed the *Gegenbauer coefficients* of f.

Proposition 2.4. *For any $f \in L^2_{d,\mathcal{I}}$, $n \in \mathbb{N}_0$, we have*

$$f \circledast E_{d,n} = \bar{c}_{d,n}\langle f, E_{d,n}\rangle_{L^2} E_{d,n}.$$

Proof. For $N \in \mathbb{N}$ we set $f_N = \sum_{k=0}^{N}\langle f, E_{d,k}\rangle_{L^2} E_{d,k}$. Then f_N converges to f in L^2. We obtain

$$\begin{aligned}&\|f \circledast E_{d,n} - \bar{c}_{d,n}\langle f, E_{d,n}\rangle_{L^2} E_{d,n}\|_{L^2}\\ &\qquad \le \|f \circledast E_{d,n} - f_N \circledast E_{d,n}\|_{L^2} + \|f_N \circledast E_{d,n} - \bar{c}_{d,n}\langle f, E_{d,n}\rangle_{L^2} E_{d,n}\|_{L^2}.\end{aligned}$$

The last summand on the right hand side is zero by the definition of f_N and Proposition 2.2. By Proposition 2.1 we obtain

$$\|f \circledast E_{d,n} - f_N \circledast E_{d,n}\|_{L^2} = \|(f - f_N) \circledast E_{d,n}\|_{L^2} \le \|f - f_N\|_{L^2}\|E_{d,n}\|_{L^2} \to 0,$$

as $N \to \infty$. □

Corollary 2.5. *For any $f \in L^2_{d,\mathcal{I}}$, $n \in \mathbb{N}_0$ we have*

$$\langle f \circledast f, E_{d,n}\rangle_{L^2} = \bar{c}_{d,n}\langle f, E_{d,n}\rangle^2_{L^2}.$$

Proof. We have

$$\begin{aligned}\langle f \circledast f, E_{d,n}\rangle_{L^2} &= (\bar{c}_{d,n})^{-1}\langle f \circledast f, E_{d,n} \circledast E_{d,n}\rangle_{L^2} = (\bar{c}_{d,n})^{-1}\|f \circledast E_{d,n}\|^2_{L^2}\\ &= (\bar{c}_{d,n})^{-1}\|\bar{c}_{d,n}\langle f, E_{d,n}\rangle_{L^2} E_{d,n}\|^2_{L^2} = \bar{c}_{d,n}\langle f, E_{d,n}\rangle^2_{L^2},\end{aligned}$$

where we used Propositions 2.2 and 2.3, equation (2.2), and Proposition 2.4 in this order. □

The following theorem gives a necessary condition for the existence of convolution roots in $L^2_{d,\mathcal{I}}$. In the interesting special case of nonnegative Gegenbauer coefficients this condition is also sufficient.

Theorem 2.6. *If a function $f \in L^2_{d,\mathcal{I}}$ can be represented as $f = g \circledast g$ for some $g \in L^2_{d,\mathcal{I}}$, then*

$$\sum_{n=0}^{\infty}(\bar{c}_{d,n})^{-1}|\langle f, E_{d,n}\rangle_{L^2}| < \infty. \tag{2.5}$$

If (2.5) holds and $\langle f, E_{d,n}\rangle_{L^2} \ge 0$ for all $n \in \mathbb{N}_0$, then there exists a $g \in L^2_{d,\mathcal{I}}$ such that $f = g \circledast g$. The coefficients of g in the Gegenbauer basis can be chosen to be nonnegative.

Proof. The Hilbert space $L^2_{d,\mathcal{I}}$ is isometric to the space ℓ^2 [24, Corollary V.4.13]. Therefore $\sum_{n\in\mathbb{N}_0} a_n E_{d,n} \in L^2_{d,\mathcal{I}}$ if and only if $(a_n)_{n\in\mathbb{N}_0} \in \ell^2$ or, equivalently,

$\sum_{n=0}^{\infty} a_n^2 < \infty$. Suppose now that f is given by $f = g \circledast g$ for some $g \in L^2_{d,\mathcal{I}}$. By Corollary 2.5 we have that

$$\langle g, E_{d,n}\rangle_{L^2} = \pm(\bar{c}_{d,n})^{-\frac{1}{2}}|\langle f, E_{d,n}\rangle_{L^2}|^{\frac{1}{2}},$$

hence

$$\sum_{n=0}^{\infty}(\bar{c}_{d,n})^{-1}|\langle f, E_{d,n}\rangle_{L^2}| < \infty.$$

For the reverse implication set $g = \sum_{n\in\mathbb{N}_0}(\bar{c}_{d,n})^{-1/2}\langle f, E_{d,n}\rangle_{L^2}^{1/2}E_{d,n}$. By assumption $g \in L^2_{d,\mathcal{I}}$ and by Corollary 2.5 we have for any $n \in \mathbb{N}_0$ that

$$\langle g \circledast g, E_{d,n}\rangle_{L^2} = \bar{c}_{d,n}\langle g, E_{d,n}\rangle_{L^2}^2 = \langle f, E_{d,n}\rangle_{L^2}.$$

With Parseval's equality [24, Theorem V.4.9] this yields the claim. □

We conclude this section with a proposition that shows that convolution products can be uniformly approximated with respect to the Gegenbauer basis $\mathcal{C}_d$.

Proposition 2.7. *If $f \in L^2_{d,\mathcal{I}}$ is given by $f = g \circledast g$ for some $g \in L^2_{d,\mathcal{I}}$, then for every permutation $\sigma : \mathbb{N} \to \mathbb{N}$, the sequence $(f_N)_{N\in\mathbb{N}}$ with $f_N = \sum_{k=0}^{N}\langle f, E_{d,\sigma(k)}\rangle_{L^2}E_{d,\sigma(k)}$ converges uniformly to f.*

Proof. Let $g_N = \sum_{k=0}^{N}\langle g, E_{d,\sigma(k)}\rangle_{L^2}E_{d,\sigma(k)}$. By Corollary 2.5 and Proposition 2.4 we have

$$\begin{aligned} f - f_N &= g \circledast g - \sum_{k=0}^{N}\bar{c}_{d,\sigma(k)}\langle g, E_{d,\sigma(k)}\rangle_{L^2}^2 E_{d,\sigma(k)} \\ &= g \circledast g - \sum_{k=0}^{N}\langle g, E_{d,\sigma(k)}\rangle_{L^2} g \circledast E_{d,\sigma(k)} = g \circledast g - g \circledast g_N = g \circledast (g - g_N). \end{aligned}$$

Now, we can apply Proposition 2.1 to the last term and use the unconditional L^2-convergence of g_N to g in order to obtain the claim. □

3. Convolution roots

Schoenberg's characterization of the classes Ψ_d is summarized in the following theorem; cf. [20].

Theorem 3.1 (Schoenberg)**.** *The class Ψ_d consists of all functions of the form*

$$\psi(\vartheta) = \sum_{n=0}^{\infty} b_{d,n}\frac{C_n^{(d-1)/2}(\cos\vartheta)}{C_n^{(d-1)/2}(1)}, \quad \text{for } \vartheta \in [0,\pi],$$

with nonnegative coefficients $b_{d,n}$, such that $\sum_{n=0}^{\infty} b_{d,n} = 1$. If $d = 1$, then

$$b_{1,0} = \frac{1}{\pi}\int_0^{\pi}\psi(\vartheta)d\vartheta \quad \text{and} \quad b_{1,n} = \frac{2}{\pi}\int_0^{\pi}\cos(n\vartheta)\psi(\vartheta)d\vartheta, \quad \text{for } n \geq 1. \tag{3.1}$$

If $d \geq 2$, then, for $n \in \mathbb{N}_0$,

$$b_{d,n} = \frac{2n+d-1}{2^{3-d}\pi}\frac{\left(\Gamma(\frac{d-1}{2})\right)^2}{\Gamma(d-1)}\int_0^{\pi}\left\{C_n^{(d-1)/2}(\cos\vartheta)\right\}(\sin\vartheta)^{d-1}\psi(\vartheta)d\vartheta. \tag{3.2}$$

For a function $\psi \in \Psi_d$, we call the associated coefficients $b_{d,n}$ as given by (3.1) or (3.2), respectively, the *d-dimensional Schoenberg coefficients* of ψ.

A function $\psi \in \Psi_d$ is *strictly positive definite* if the inequality in (1.1) is strict for all systems of pairwise distinct points, unless all the coefficients are zero. A function $\psi \in \Psi_d$ for $d \geq 2$ is strictly positive definite if and only if its Schoenberg coefficients $b_{d,n}$ are strictly positive for infinitely many even and infinitely many odd integers n [5]. The corresponding result for Ψ_∞ was derived in [15]. Characterizations of the strictly positive definite functions in Ψ_1 in terms of nonzero Schoenberg coefficients are available in [16, 17].

We prove the following result, which is slightly more detailed than Theorem 1.1.

Theorem 3.2. *For any $\psi \in \Psi_d$ there exists a function $g \in L^2_{d,\mathcal{I}}$ such that*

$$\psi(\theta(u,v)) = (g \circledast g)(u,v), \quad \text{for all } u,v \in \mathbb{S}^d,$$

and g has nonnegative Gegenbauer coefficients.

Proof. First, let $d \geq 2$, $\psi \in \Psi_d$. The nonnegative Schoenberg coefficients of ψ are connected to the Gegenbauer coefficients of $\psi(\theta(\cdot,\cdot))$ via

$$\begin{aligned} b_{d,n} &= \frac{2n+d-1}{2^{3-d}\pi} \frac{(\Gamma(\frac{d-1}{2}))^2}{\Gamma(d-1)} \int_0^\pi C_n^{(d-1)/2}(\cos\vartheta)(\sin\vartheta)^{d-1}\psi(\vartheta)d\vartheta \\ &= \frac{2n+d-1}{2^{3-d}\pi} \frac{(\Gamma(\frac{d-1}{2}))^2}{\Gamma(d-1)} \left(2\pi\sigma_d \prod_{k=2}^{d-1} \int_0^\pi (\sin\vartheta)^{k-1} d\vartheta\right)^{-1} \\ &\qquad \times \int_{\mathbb{S}^d\times\mathbb{S}^d} C_n^{(d-1)/2}(\langle u,v\rangle)\psi(\theta(u,v))dudv \\ &= \frac{(\Gamma(\frac{d-1}{2}))^2\Gamma(\frac{d}{2})(d-1)}{\Gamma(d-1)2^{4-d}\pi^{(d+1)/2}} (\bar{c}_{d,n})^{-1}\langle E_{d,n}, \psi(\theta(\cdot,\cdot))\rangle_{L^2}. \end{aligned}$$

The quotient in the previous line is positive and depends only on d. We denote it by α_d. In particular, $\langle E_{d,n}, \psi(\theta(\cdot,\cdot))\rangle_{L^2} \geq 0$ for all $n \in \mathbb{N}_0$. We have

$$\frac{C_n^{(d-1)/2}(\langle\cdot,\cdot\rangle)}{C_n^{(d-1)/2}(1)} = \sigma_d \bar{c}_{d,n} E_{d,n},$$

hence

$$\psi(\theta(\cdot,\cdot)) = \alpha_d\sigma_d \sum_{n=0}^\infty \langle E_{d,n}, \psi(\theta(\cdot,\cdot))\rangle_{L^2} E_{d,n}.$$

By Theorem 3.1

$$\begin{aligned} 1 = \sum_{n=0}^\infty b_{n,d} = \alpha_d \sum_{n=0}^\infty (\bar{c}_{d,n})^{-1}\langle E_{d,n}, \psi(\theta(\cdot,\cdot))\rangle_{L^2} \\ = \alpha_d \sum_{n=0}^\infty (\bar{c}_{d,n})^{-1}|\langle E_{d,n}, \psi(\theta(\cdot,\cdot))\rangle_{L^2}|; \end{aligned}$$

hence Theorem 2.6 yields the claim. For $d = 1$ we have

$$b_{1,n} = \begin{cases} 1/(2\pi)\langle E_{1,n}, \psi(\theta(\cdot,\cdot))\rangle_{L^2}, & \text{if } n = 0, \\ \sqrt{2}/(2\pi)\langle E_{1,n}, \psi(\theta(\cdot,\cdot))\rangle_{L^2}, & \text{if } n \geq 1; \end{cases}$$

hence we can apply the same arguments as above. □

Remark 3.3. For a function $\psi \in \Psi_{d+k} \subset \Psi_d$ for some $k \geq 1$, Theorem 3.2 yields spherical convolution roots $g_{d+k} \in L^2_{d+k,\mathcal{I}}$ and $g_d \in L^2_{d,\mathcal{I}}$ with respect to the convolution in $\mathbb{S}^{d+k}$ and $\mathbb{S}^d$, respectively. The associated functions $\bar{g}_{d+k}$, $\bar{g}_d$ are both defined on $[0,\pi]$, and one would hope for a simple functional relationship between them, but it remains elusive thus far. However, on the level of Schoenberg coefficients, the functions g_{d+2} and g_d are easily put in relation using [11, Corollary 3].

Let $\psi \in \Psi_d$. The construction in the proofs of Theorems 2.6 and 3.2 shows that the class $\mathcal{G}_d(\psi)$ of all spherical convolution roots $g \in L^2_{d,\mathcal{I}}$ of ψ is given by all functions $g \in L^2_{d,\mathcal{I}}$, whose Gegenbauer coefficients are given by

$$\left(\alpha_d^{-\frac{1}{2}} \sigma_n b_{d,n}^{\frac{1}{2}}\right)_{n\in\mathbb{N}_0}, \tag{3.3}$$

where $(b_{d,n})_{n\in\mathbb{N}_0}$ are the Schoenberg coefficients of ψ and $(\sigma_n)_{n\in\mathbb{N}_0}$ is a sequence with $\sigma_n \in \{-1,1\}$; cf. Figure 1. In Theorem 3.2 we identify a unique convolution root by setting $\sigma_n = 1$ for all $n \in \mathbb{N}_0$. This choice resolves the identifiability issue when inferring the kernel of Lévy based models for star-shaped random particles from their covariance or correlation structure as mentioned in Section 1. See also [12, 27].

We conclude the section by using the convolution representation to calculate the Schoenberg coefficients of the function

$$\iota_d : [0,\pi] \to \mathbb{R}, \vartheta \mapsto \frac{1}{\nu_d(r)} \overline{\mathbb{1}_{\{\theta(\cdot,\cdot)\leq r\}} \circledast \mathbb{1}_{\{\theta(\cdot,\cdot)\leq r\}}}(\vartheta),$$

where $r \in (0,\pi/2]$ and ν_d is the normalizing constant ensuring that $\iota_d(0) = 1$. Here, $\mathbb{1}_A$ denotes the indicator function of a set A. The convolution is taken in $\mathbb{S}^d \times \mathbb{S}^d$. It is a short calculation to show that $\nu_1(r) = 2r$. For $d \geq 2$ the normalizing constant is given by

$$\nu_d(r) = \sigma_{d-1} \int_0^r (\sin\vartheta)^{d-1} d\vartheta. \tag{3.4}$$

The function ι_2 has been calculated explicitly in [23]. Estrade and Istas [8] provide a recursive formula for the functions ι_d, $d \geq 2$.

Lemma 3.4. *Let $r \in (0,\pi/2]$. The function $\mathbb{1}_{\{\theta(\cdot,\cdot)\leq r\}} \in L^2_{d,\mathcal{I}}$ has Gegenbauer coefficients $\{\omega_{d,n}\}_{n\in\mathbb{N}_0}$ given, for $n \geq 1$, by*

$$\omega_{d,n} = c_{d,n}\sigma_d\sigma_{d-1}\frac{d-1}{n(n+d-1)}(\sin(r))^d C_{n-1}^{(d+1)/2}(\cos(r)), \quad \textit{for } d \geq 2,$$

and $\omega_{1,n} = (2\sqrt{2}/n)\sin(nr)$. Finally, $\omega_{d,0} = \nu_d(r)$, where $\nu_d(r)$ is given in (3.4).

Proof. Suppose first that $d \geq 2$. We have

$$\begin{aligned}
\langle \mathbb{1}_{\{\theta(\cdot,\cdot)\leq r\}}, E_{d,n}\rangle_{L^2_d} &= c_{d,n} \int_{\mathbb{S}^d}\int_{\mathbb{S}^d} \mathbb{1}_{\{\theta(u,v)\leq r\}} C_n^{(d-1)/2}(\langle u,v\rangle) du dv \\
&= c_{d,n}\sigma_d^2 \left(\int_0^\pi (\sin\vartheta)^{d-1} d\vartheta\right)^{-1} \int_0^\pi \mathbb{1}_{\{\vartheta\leq r\}} C_n^{(d-1)/2}(\cos\vartheta)(\sin\vartheta)^{d-1} d\vartheta \\
&= c_{d,n}\sigma_d\sigma_{d-1} \int_{\cos(r)}^1 C_n^{(d-1)/2}(u)(1-u^2)^{(d-2)/2} du.
\end{aligned}$$

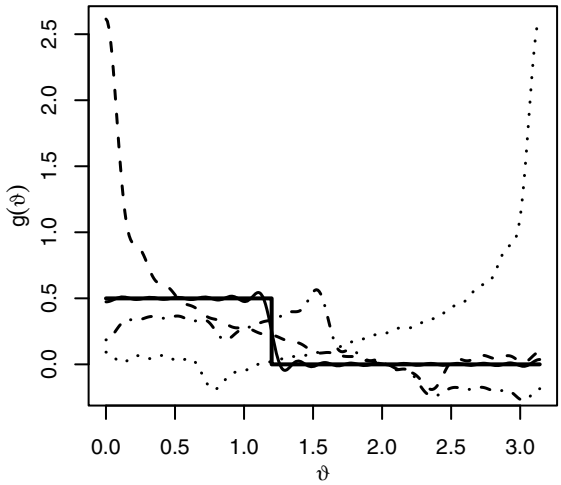

FIGURE 1. Different convolution roots g of $\iota_2(r)$ for $r = 1.2$. The solid lines display the function $\nu_d(1.2)^{-1/2}\mathbb{1}_{\{\vartheta\le 1.2\}}$ and its approximation by the first 32 Gegenbauer polynomials. The dashed line is the convolution root with nonnegative Gegenbauer coefficients. The dotted line represents the convolution root with $\sigma_n = (-1)^n$, whereas the dash-dotted line has $\sigma_n = (-1)^{[n/2]}$, with $(\sigma_n)_{n\in\mathbb{N}_0}$ as in (3.3).

Using $c_{d,0} = \sigma_d^{-1}$, the formula for $n = 0$ follows. By [6, 18.9.20] we have for $n \ge 1$

$$\frac{d}{dx}\left((1-x^2)^{d/2}C_{n-1}^{(d+1)/2}(x)\right) = -\frac{n(n+d-1)}{d-1}(1-x^2)^{(d-2)/2}C_n^{(d-1)/2}(x), \tag{3.5}$$

which implies the lemma. The case $d = 1$ is a simple calculation. □

Using the relation between the Gegenbauer and the Schoenberg coefficients calculated in the proof of Theorem 3.2 we obtain the following corollary.

Corollary 3.5. *The function ι_d is in Ψ_d. For $d \ge 2$ its Schoenberg coefficients are given by*

$$b_{d,0} = \frac{\nu_d(r)}{\sigma_d^2}\frac{\Gamma(\frac{d-1}{2})^2\Gamma(\frac{d}{2})(d-1)}{\Gamma(d-1)2^{4-d}\pi^{(d+1)/2}},$$

and, for $n \ge 1$,

$$b_{d,n} = \gamma_d(r)(2n+d-1)C_n^{(d-1)/2}(1)\left(\frac{C_{n-1}^{(d+1)/2}(\cos r)}{C_{n-1}^{(d+1)/2}(1)}\right)^2,$$

where

$$\gamma_d(r) = \frac{1}{\nu_d(r)}\frac{\Gamma(\frac{d-1}{2})^2 2^{d-2}\pi^{(d-1)/2}}{d^2\Gamma(\frac{d}{2})}(\sin r)^{2d}.$$

For $d = 1$, we have $b_{1,0} = r/(4\pi^3)$ and $b_{1,n} = \sqrt{2}\sin^2(nr)/(rn^2\pi^2)$ for $n \ge 1$.

This example illustrates that the convolution root constructed in Theorem 3.2 may not be the most natural one. The Gegenbauer coefficients of $\nu_d(r)^{-1/2}\times \mathbb{1}_{\{\theta(\cdot,\cdot)\leq r\}}$ take both positive and negative signs; cf. Lemma 3.4. Hence, it is not the convolution root of ι_d that results from the construction in Theorem 3.2; cf. Figure 1. The function ι_d is an example of a member of Ψ_d that is supported on a spherical cap of radius $2r$. If we would like to have a convolution root that is supported on a spherical cap of radius r, such as $\nu_d(r)^{-1/2}\mathbb{1}_{\{\theta(\cdot,\cdot)\leq r\}}$ for ι_d, it may not be suitable to choose all coefficients of the convolution root nonnegative. In the Euclidean case, the existence of convolution roots with half-support, the so-called *Boas-Kac roots*, is discussed in [7], building on the classical result of Boas and Kac [3]. It remains an open problem whether Boas-Kac roots always exist for functions in Ψ_d.

4. Differentiability

4.1. **Proof of Theorem 1.2.** We denote by $\tilde{\Psi}_d$ the space of all continuous functions $\varphi : [0,\pi] \to \mathbb{R}$ which are such that the function $\varphi(\theta(\cdot,\cdot)) : \mathbb{S}^d \times \mathbb{S}^d \to \mathbb{R}$ is positive definite. The difference between the spaces Ψ_d and $\tilde{\Psi}_d$ is that the members $\psi \in \Psi_d \subset \tilde{\Psi}_d$ are additionally required to fulfill $\psi(0) = 1$. Theorems 3.1 and 3.2 also hold for the class $\tilde{\Psi}_d$ with the obvious modification that we need to require $\sum_{n=0}^{\infty} b_{d,n} < \infty$ instead of $\sum_{n=0}^{\infty} b_{d,n} = 1$ for the Schoenberg coefficients in the former.

For the proof of Theorem 1.2 on the differentiability of positive definite functions on spheres we show the following proposition, which can be applied iteratively to yield the assertion.

Proposition 4.1. *Let $d \geq 1$, $\psi \in \tilde{\Psi}_{d+2}$. Then ψ is continuously differentiable in $(0,\pi)$ and its derivative can be written as*

$$\psi'(\vartheta) = \frac{1}{\sin\vartheta}\left(f_1(\vartheta) - f_2(\vartheta)\right),$$

where $f_1, f_2 \in \tilde{\Psi}_d$.

Proof. By [6, 18.9.19] the derivative of C_n^α for $\alpha > 0$ and $n \geq 1$ is given by

$$\frac{d}{dx}C_n^\alpha(x) = 2\alpha C_{n-1}^{\alpha+1}(x). \tag{4.1}$$

We assume first that $d \geq 2$. As $\tilde{\Psi}_d \supset \tilde{\Psi}_{d+2}$ we can write ψ as

$$\psi(\vartheta) = \sum_{n=0}^{\infty} b_{d,n}\frac{C_n^{(d-1)/2}(\cos\vartheta)}{C_n^{(d-1)/2}(1)}, \quad \vartheta \in [0,\pi],$$

with nonnegative coefficients $b_{d,n}$ such that $\sum_{n=0}^{\infty} b_{d,n} < \infty$; see Theorem 3.1. For $N \in \mathbb{N}$, $\vartheta \in [0,\pi]$ we define

$$\psi_N(\vartheta) = \sum_{n=0}^{N} b_{d,n}\frac{C_n^{(d-1)/2}(\cos\vartheta)}{C_n^{(d-1)/2}(1)}.$$

By Proposition 2.7 ψ_N converges uniformly to ψ. Let $\vartheta \in (0,\pi)$. By (4.1), the derivative of ψ_N is given by

$$\begin{aligned}\psi_N'(\vartheta) &= \sum_{n=1}^{N} b_{d,n}(d-1)\frac{C_{n-1}^{(d+1)/2}(\cos\vartheta)}{C_n^{(d-1)/2}(1)}(-\sin\vartheta)\\ &= \frac{-1}{\sin\vartheta}\sum_{n=1}^{N} b_{d,n}\frac{1}{C_n^{(d-1)/2}(1)}\left(\frac{(n+d-2)(n+d-1)}{2n+d-1}C_{n-1}^{(d-1)/2}(\cos\vartheta)\right.\\ &\qquad\left.-\frac{n(n+1)}{2n+d-1}C_{n+1}^{(d-1)/2}(\cos\vartheta)\right)\\ &= \frac{1}{\sin\vartheta}\sum_{n=1}^{N} b_{d,n}\frac{n(n+d-1)}{2n+d-1}\left(\frac{C_{n+1}^{(d-1)/2}(\cos\vartheta)}{C_{n+1}^{(d-1)/2}(1)}-\frac{C_{n-1}^{(d-1)/2}(\cos\vartheta)}{C_{n-1}^{(d-1)/2}(1)}\right),\end{aligned}$$

where we used (2.3) and

$$\begin{aligned}C_n^{(d+1)/2}(\cos\vartheta)(\sin\vartheta)^2 &= \frac{(n+d-1)(n+d)}{(d-1)(2n+d+1)}C_n^{(d-1)/2}(\cos\vartheta)\\ &\qquad-\frac{(n+1)(n+2)}{(d-1)(2n+d+1)}C_{n+2}^{(d-1)/2}(\cos\vartheta);\end{aligned}$$

see [6, equation (18.9.8)]. Therefore

$$\begin{aligned}(\sin\vartheta)\psi_N'(\vartheta) &= -b_{d,1}\frac{d}{d+1}\\ &\quad+\sum_{n=0}^{N}\left(\frac{n(n+d-1)}{2n+d-1}b_{d,n}-\frac{(n+2)(n+d+1)}{2n+d+3}b_{d,n+2}\right)\frac{C_{n+1}^{(d-1)/2}(\cos\vartheta)}{C_{n+1}^{(d-1)/2}(1)}\\ &\quad+\sum_{n=N-1}^{N} b_{d,n+2}\frac{(n+2)(n+d+1)}{2n+d+3}\frac{C_{n+1}^{(d-1)/2}(\cos\vartheta)}{C_{n+1}^{(d-1)/2}(1)}.\end{aligned}$$

The last term in the above equation converges to zero uniformly in ϑ as $N\to\infty$ by [11, Corollary 4] and Lemma 4.2. We will omit it in the sequel. Using [11, Corollary 3(b)], we obtain

$$\begin{aligned}&\frac{n(n+d-1)}{2n+d-1}b_{d,n}-\frac{(n+2)(n+d+1)}{2n+d+3}b_{d,n+2}\\ &\qquad= \frac{dn}{n+d}b_{d+2,n}-\frac{d(2n+d+1)(n+2)}{(2n+d+3)(n+d)}b_{d,n+2}.\end{aligned}$$

Hence,

$$\begin{aligned}(\sin\vartheta)\psi_N'(\vartheta) &= d\sum_{n=0}^{N}\frac{n}{n+d}b_{d+2,n}\frac{C_{n+1}^{(d-1)/2}(\cos\vartheta)}{C_{n+1}^{(d-1)/2}(1)}\\ &\quad-d\sum_{n=1}^{N+2}\frac{(2n+d-3)n}{(2n+d-1)(n+d-2)}b_{d,n}\frac{C_{n-1}^{(d-1)/2}(\cos\vartheta)}{C_{n-1}^{(d-1)/2}(1)}.\end{aligned}$$

We set $\beta_0^{(1)}=0$,

$$\beta_n^{(1)} = d\frac{n-1}{n+d-1}b_{d+2,n-1},\quad \text{for } n\ge 1,$$

and

$$\beta_n^{(2)} = d\frac{(2n+d-1)(n+1)}{(2n+d+1)(n+d-1)}b_{d,n+1}, \quad \text{for } n \geq 0.$$

The sequences $\{\beta_n^{(i)}\}_{n\in\mathbb{N}_0}$, $i = 1, 2$, are nonnegative and summable by assumption. Therefore they are the Schoenberg coefficients of some functions f_1, $f_2 \in \tilde{\Psi}_d$. By Proposition 2.7 their partial Gegenbauer sums converge uniformly, which yields the claim.

If $d = 1$, the proof uses the same arguments with [11, Corollary 3(a)] instead of [11, Corollary 3(b)]. The Schoenberg coefficients of the functions f_1, f_2 are then given by $\beta_n^{(1)} = ((n-1)/n)b_{3,n-1}$, $\beta_n^{(2)} = b_{1,n+1}$, for $n \geq 1$, and $\beta_0^{(1)} = 0$, $\beta_0^{(2)} = (1/2)b_{1,1}$. □

Lemma 4.2. *Let $(\alpha_n)_{n\in\mathbb{N}}$ be an increasing sequence converging to 1 such that the sequence $(\alpha_n^n)_{n\in\mathbb{N}}$ is bounded away from 0. Suppose that $\sum_{n=1}^{\infty} b_n < \infty$ for some sequence $(b_n)_{n\in\mathbb{N}}$ of nonnegative numbers. If*

$$b_n \geq \alpha_n b_{n+1}, \quad \textit{for all } n \in \mathbb{N},$$

then $n\, b_n \to 0$ as $n \to \infty$.

Proof. Let $(\alpha_n^n)_{n\in\mathbb{N}}$ be bounded below by $C > 0$. Let $\varepsilon > 0$ and choose n_0 such that $\sum_{k=n+1}^{m} b_k < \varepsilon$ for all $m > n > n_0$. With $m = 2n$ we obtain

$$\varepsilon > \sum_{k=n+1}^{2n} b_k \geq \sum_{k=n+1}^{2n} \prod_{j=k}^{2n-1} \alpha_j b_{2n} \geq \sum_{k=n+1}^{2n} (\alpha_n)^{2n-k} b_{2n}$$
$$\geq \alpha_n^{2n} n\, b_{2n} \geq C^2\, n\, b_{2n} \geq 0.$$

Using the same argument for $m = 2n + 1$ yields the claim. □

4.2. **Optimality of Theorem 1.2.** In this section we show that Theorem 1.2 is optimal for all odd dimensions using similar ideas as in [10].

Proposition 4.3. *Let d be an odd integer. Then there exists a function $\psi \in \Psi_d$ whose derivative of order $(d-1)/2$ is not continuously differentiable.*

We are not aware of a function $\psi \in \Psi_2$ with discontinuous derivative. If such a function were available, our method would immediately also yield the optimality of the differentiability result in even dimensions.

For the proof of Proposition 4.3, we introduce a *turning bands operator* for isotropic positive definite functions on spheres in analogy to the Euclidean case, where the turning bands operator originates in the work of Matheron [14]. Let $\beta = (\beta_n)_{n\in\mathbb{N}_0}$ be a sequence of real numbers. For an integer $k \in \mathbb{Z}$ we define the sequence $\beta \circ \tau_k$ as follows. If $k > 0$ its members are

$$(\beta \circ \tau_k)_n = \begin{cases} 0, & \text{if } n < k, \\ \beta_{n-k}, & \text{if } n \geq k \end{cases}$$

for $n \in \mathbb{N}_0$. If $k \leq 0$ we put $(\beta \circ \tau_k)_n = \beta_{n-k}$ for all $n \in \mathbb{N}_0$. Let $d \geq 1$ be an integer. For a summable sequence $\beta = (\beta_n)_{n\in\mathbb{N}}$ of nonnegative numbers β_n we define $\psi_d(\beta, \vartheta)$ for $\vartheta \in [0, \pi]$ as

$$\psi_d(\beta, \vartheta) = \sum_{n=0}^{\infty} \beta_n \frac{C_n^{(d-1)/2}(\cos\vartheta)}{C_n^{(d-1)/2}(1)} \in \tilde{\Psi}_d.$$

Proposition 4.4. *Let $d \geq 1$ be an integer and let $\beta = (\beta_n)_{n\in\mathbb{N}}$ be a summable sequence of nonnegative numbers β_n. Then, for all $r \in [0, \pi]$,*

$$\psi_d(\beta, r) = \beta_0 + \cos r \ \psi_{d+2}(\beta \circ \tau_{-1}, r) + \frac{1}{d} \sin r \ \psi'_{d+2}(\beta \circ \tau_{-1}, r) \tag{4.2}$$

and

$$\frac{1}{d}(\sin r)^d \ \psi_{d+2}(\beta \circ \tau_{-1}, r) = \int_0^r (\sin \vartheta)^{d-1}(\psi_d(\beta, \vartheta) - \beta_0) d\vartheta. \tag{4.3}$$

Proof. Suppose first that $d \geq 2$. Using Proposition 2.7, (3.5), and (2.3) we obtain

$$\begin{aligned}\int_0^r (\sin \vartheta)^{d-1} \psi_d(\beta, \vartheta) d\vartheta &= \sum_{n=0}^{\infty} \beta_n \int_0^r (\sin \vartheta)^{d-1} \frac{C_n^{(d-1)/2}(\cos \vartheta)}{C_n^{(d-1)/2}(1)} d\vartheta \\ &= \beta_0 \int_0^r (\sin \vartheta)^{d-1} d\vartheta + \frac{1}{d}(\sin r)^d \sum_{n=1}^{\infty} \beta_n \frac{C_{n-1}^{(d+1)/2}(\cos r)}{C_{n-1}^{(d+1)/2}(1)},\end{aligned}$$

which implies (4.3). Differentiating both sides of (4.3) with respect to r yields (4.2). The case $d = 1$ can be shown using the same arguments. □

Lemma 4.5. *Let $d \geq 1$ be an integer and let $\beta = (\beta_n)_{n\in\mathbb{N}}$ be a summable sequence of nonnegative numbers β_n. For any $k \in \mathbb{Z}$ the function $\psi_d(\beta \circ \tau_k, \cdot)$ is continuously differentiable if and only if the same holds true for $\psi_d(\beta, \cdot)$.*

Proof. The proof of Theorem 1.2 shows that the differentiability of a function $\psi_d(\beta, \cdot)$ depends only on the nonnegativity and asymptotic properties of the sequence $(\beta_n)_{n\in\mathbb{N}_0}$. □

Proof of Proposition 4.3. Let $c \in (0, \pi)$. Then the function

$$\psi(\vartheta) = \max\left\{0, \left(1 - \frac{\vartheta}{c}\right)\right\}, \quad \vartheta \in [0, \pi],$$

belongs to the class Ψ_1 as can be shown by elementary arguments. Its first derivative does not exist at the point $\vartheta = c$. Let $\beta = (\beta_n)_{n\in\mathbb{N}_0}$ be the sequence of 1-dimensional Schoenberg coefficients of ψ. Let $d \geq 3$ be an odd integer. By (4.3) and Lemma 4.5, the function $\psi_d(\beta \circ \tau_{-(d-1)/2}, \vartheta) \in \Psi_d$ and its derivative of order $1 + (d-1)/2$ do not exist at $\vartheta = c$. □

The truncated power functions $\psi(\vartheta) = \max\{0, (1-\vartheta/c)^\tau\}$ were studied in detail in [2]. The authors were able to show that they belong to Ψ_d if $\tau \geq (d+1)/2$ for $d = 3, 5, 7$ and conjectured the result for all dimensions. Theorem 1.2 immediately shows the necessity of the condition for all odd dimensions.

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