



Strict Positive Definiteness of Convolutional and Axially Symmetric Kernels on d -Dimensional Spheres

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Abstract

The paper introduces new sufficient conditions of strict positive definiteness for kernels on d -dimensional spheres which are not radially symmetric but possess specific coefficient structures. The results use the series expansion of the kernel in spherical harmonics. The kernels either have a convolutional form or are axially symmetric with respect to one axis. The given results on convolutional kernels generalise the result derived by Chen et al. (Proc Am Math Soc 131:2733–2740, 2003) for radial kernels.

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1 Introduction

Spherical approximation is a topic of immense interest and the use of positive definite spherical basis functions has recently been discussed in a tremendous number of publications [8, 14, 16, 23]. Most of the known results are for isotropic positive definite kernels, which are kernels that only depend on the geodesic distance of their arguments. Isotropic kernels are the generalisation of the radial basis function method to the sphere and therefore referred to in approximation theory as spherical radial basis functions (see [16] and references therein). They are also of importance in statistics where they occur as correlation functions of homogeneous random fields on spheres [18, 19].

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In Euclidean space the study of general (non radial) kernel methods has gained importance, see for example [13]. Our paper aims to provide a starting point for such general kernel methods on spheres by stating a general series representation of kernels on the sphere and first establishing connections between geometric properties of the kernel (like isotropy or axial symmetry) and the series representation. Then positive definiteness and strict positive definiteness of such kernels are studied.

We summarise the existing results on kernel methods, these mainly focus on the 2-sphere. Recently, the use of (non-isotropic) kernels on the 2-sphere was suggested and applied for the approximation of global data in [5, 11, 12, 24], the latter three papers using non isotropic kernels on the sphere or the sphere cross-time. Conditions that ensure strict positive definiteness of axially-symmetric kernels on the 2-sphere were proven in [6]. These results are in this paper generalised to d -dimensional spheres and additional necessary conditions are proven.

The second type of non-radial kernels we study are convolutional kernels which have for example been described in [7, 25], where the second reference includes conditions for strict positive definiteness similar to the ones we will present but only for the case of the two-sphere.

The new results we present refer to higher-dimensional spheres, too, these have to be studied separately since the basis functions used for the description of the kernels have a more complicated structure in higher dimensions. Also we simplify the technique of the proof for the convolutional kernels by not using a fixed basis of the spherical harmonics.

The results for convolutional kernels are closely connected to the ones known for isotropic kernels and easier to verify than the abstract results for axially symmetric kernels. However, the convolutional kernels contain a subclass of the axially symmetric kernels which allows the use of the more applicable results for the construction of axially symmetric kernels.

We will briefly summarise the needed definitions in the first section and then, starting from a general form of the kernel, state conditions which ensure certain properties of the kernel, like axial symmetry, convolutional form and invariance under parity. In the third section, we give sufficient conditions for axially symmetric kernels to be positive definite and strictly positive definite and add some necessary conditions. In the fourth part of this paper we generalise the result of Chen et al. [8] on radial kernels to convolutional kernels deriving sufficient conditions on strict positive definiteness and finally study the special case of the circle in the last section.

1.1 Problem Description and Background

We focus on interpolation problems on the d -sphere

$$\mathbb{S}^{d-1} = \left\{ \xi \in \mathbb{R}^d \mid \xi_1^2 + \xi_2^2 + \cdots + \xi_d^2 = 1 \right\}, \quad d \geq 2,$$

where a finite set of distinct data sites $\mathcal{E} \subset \mathbb{S}^{d-1}$ and values $f(\xi) \in \mathbb{C}$, $\xi \in \mathcal{E}$, of a possibly elsewhere unknown function f on the sphere are given.

The approximant is formed as a linear combination of kernels

$$K : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \rightarrow \mathbb{C}.$$

Taking the form

$$s_f(\zeta) = \sum_{\xi \in \mathcal{E}} c_\xi K(\zeta, \xi), \quad \zeta \in \mathbb{S}^{d-1}, \tag{1}$$

the problem of finding such an approximant s_f satisfying

$$s_f(\xi) = f(\xi), \quad \forall \xi \in \mathcal{E}, \tag{2}$$

is uniquely solvable under certain conditions on K . We assume all the kernels to be Hermitian, meaning they satisfy $K(\xi, \zeta) = \overline{K(\zeta, \xi)}$, so that the positive definiteness of the kernel will ensure the solvability of the interpolation problem for arbitrary data sets.

Definition 1 A Hermitian kernel $K : \Omega \times \Omega \rightarrow \mathbb{C}$ is called positive definite on Ω if the matrix $K_{\mathcal{E}} = \{K(\xi, \zeta)\}_{\xi, \zeta \in \mathcal{E}}$ is positive semi-definite on $\mathbb{C}^{|\mathcal{E}|}$ for arbitrary finite sets of distinct points $\mathcal{E} \subset \Omega$.

The kernel is strictly positive definite if $K_{\mathcal{E}}$ is a positive definite matrix on $\mathbb{C}^{|\mathcal{E}|}$ for arbitrary finite sets of distinct points \mathcal{E} .

We assume that K is square-integrable and can be represented as a series

$$K(\xi, \zeta) = \sum_{j, j'=0}^{\infty} \sum_{k=1}^{N_{j,d}} \sum_{k'=1}^{N_{j',d}} a_{j, j', k, k'} Y_j^k(\xi) \overline{Y_{j'}^{k'}(\zeta)}, \quad \forall \xi, \zeta \in \mathbb{S}^{d-1}, \tag{3}$$

where the Y_j^k form an orthonormal basis of the eigenfunctions of the Laplace–Beltrami operator on the sphere and the corresponding eigenvalues increase with j . The $a_{j, j', k, k'}$ are complex numbers and square-summable as a consequence of the square-integrability of K . The eigenfunctions are the solutions of the eigenfunction problem

$$\lambda f + \Delta f = 0,$$

where Δ is the Laplace–Beltrami operator on the sphere. For example on the 2-sphere such a basis can take the form

$$Y_j^k(\xi) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{2j+1}{2} \frac{(j-k)!}{(j+k)!}} P_j^k(\cos(\theta)) e^{ik\varphi}, \tag{4}$$

where $(\theta, \varphi) \in [0, 2\pi) \times [0, \pi)$ are the polar coordinates representing ξ , and P_j^k are the associated Legendre polynomials (see for example 8.1.2, [1]).

The eigenfunctions corresponding to the eigenvalues $\lambda_j = j(j + d - 1)$ are spherical harmonics and the number of eigenfunctions corresponding to the eigenvalue λ_j is denoted by $N_{j,d}$. The numbers are given by $N_{0,d} = 1$,

$$N_{j,d} = \frac{(2j + d - 2)(j + d - 3)!}{j!(d - 2)!}.$$

We will denote the space of all spherical harmonics corresponding to the eigenvalue λ_j by $H_j := \text{span}\{Y_j^k \mid k = 1, \dots, N_{j,d}\}$. Additionally we will use the following estimate which holds for any orthonormal basis and is a direct consequence of the Poisson summation formula ([3], Equation (2.35))

$$|Y_j^k(\xi)| \leq \sqrt{\frac{N_{j,d}}{\sigma_{d-1}}}, \quad \forall \xi \in \mathbb{S}^{d-1}, \tag{5}$$

where σ_{d-1} is the surface area of \mathbb{S}^{d-1} .

It is well known and used in the characterisation above that every function in $L^2(\mathbb{S}^{d-1})$ can be represented as a spherical harmonic expansion of the form

$$g(\xi) = \sum_{j=0}^{\infty} \sum_{k=1}^{N_{j,d}} \hat{g}_{j,k} Y_j^k(\xi), \quad \text{with } \hat{g}_{j,k} = \int_{\mathbb{S}^{d-1}} g(\zeta) \overline{Y_j^k(\zeta)} d\sigma(\zeta), \tag{6}$$

where $d\sigma$ is the surface area measure on \mathbb{S}^{d-1} . For this expansion the Parseval equation for spherical harmonics holds ([3], (2.143)):

$$\|g\|_{L^2(\mathbb{S}^{d-1})}^2 = \sum_{j=0}^{\infty} \sum_{k=1}^{N_{j,d}} |\hat{g}_{j,k}|^2.$$

2 Kernels with Special Coefficient Structure

We now fix a basis for our space of spherical harmonics such that the kernels which are still Hermitian and square-integrable are represented as in (3). We demonstrate in this section how geometric properties of the kernel and the coefficient structure of the series representation are connected. Thereby imposing certain conditions on the structure of the coefficients allows us to focus on kernels with specific properties in the next sections.

The case studied most often is assuming that the kernel is isotropic [26], which means it only depends on the distance of its two arguments and not on their position on the sphere. The coefficients of an isotropic positive definite kernel given in the form (3) satisfy

$$a_{j,j',k,k'} = c_j \delta_{j',j} \delta_{k,k'} \geq 0$$

as stated by Schoenberg [26]. A characterisation of the strictly positive definite kernels of this form was presented by Chen et al. in [8].

Recently, a sufficient condition for axially symmetric kernels on the two-sphere to be strictly positive definite was presented in [6]. The axially symmetric kernels on \mathbb{S}^2 do depend on the difference in longitude of the two inputs ξ, ζ and their individual values of latitude. The coefficients of these kernels satisfy

$$a_{j,j',k,k'} = c_k(j, j') \delta_{k,k'},$$

where the basis of the spherical harmonics on the 2-sphere is chosen as (4). The condition was first stated in [17].

For the study of properties of the kernel we need the kernel of the form (3) to be uniquely recoverable from its Fourier expansion on $\mathbb{S}^{d-1} \times \mathbb{S}^{d-1}$ we also require the series to be absolutely summable. Therefore we start by establishing that the latter implies the former.

Lemma 1 *Let K be a kernel of the form (3). If*

$$\sum_{j,j'=0}^{\infty} \sum_{k,k'=1}^{N_{j,d},N_{j',d}} |a_{j,j',k,k'}| \sqrt{\frac{N_{j,d}N_{j',d}}{\sigma_{d-1}^2}} < \infty, \tag{7}$$

then, for each combination of $j, j' \in \mathbb{N}_0, 1 \leq k \leq N_{j,d}, 1 \leq k' \leq N_{j',d}$, the coefficients $a_{j,j',k,k'}$ can be uniquely determined by

$$a_{j,j',k,k'} = \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} K(\xi, \zeta) Y_j^k(\xi) \overline{Y_{j'}^{k'}(\zeta)} d\sigma(\xi) d\sigma(\zeta). \tag{8}$$

Proof The result follows by inserting the kernel representation (3) into (8) and then using the estimate (5) to exchange the order of summation and integration since it implies absolute summability. \square

We note that any kernel defined using coefficients satisfying property (7) will be continuous, as the upper bound is absolutely summable and all basis function are continuous. We will from now on refer to series kernels given in the form (3) which satisfy (7) simply as kernels with property (7).

First we note

Lemma 2 *Let K be a kernel with property (7). It is Hermitian if and only if*

$$a_{j,j',k,k'} = \overline{a_{j',j,k',k}} \tag{9}$$

for all possible choices $j, j' \in \mathbb{N}$ and $1 \leq k \leq N_{j,d}, 1 \leq k' \leq N_{j',d}$.

Proof Assuming K is Hermitian implies that

$$\overline{a_{j',j,k',k}} = \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} \overline{K(\xi, \zeta)} \overline{Y_{j'}^{k'}(\xi)} Y_j^k(\zeta) d\sigma(\xi) d\sigma(\zeta) = a_{j,j',k,k'}$$

according to (8). The other direction follows from representation (3). □

Besides axially symmetric kernels we are interested in kernels which are referred to as convolutional kernels. For a fixed basis of spherical harmonics these are expressed as kernels with an eigenvalue block structure but we give a non basis dependent definition.

Lemma 3 *A Hermitian kernel $K \in L^2(\mathbb{S}^{d-1} \times \mathbb{S}^{d-1})$ of the form (3) satisfies*

$$\int_{\mathbb{S}^{d-1}} K(\xi, \zeta) \overline{Y(\xi)} d\sigma(\xi) \in H_j, \quad \forall Y \in H_j,$$

if and only if

$$a_{j,j',k,k'} = \delta_{j,j'} d_j(k, k').$$

Proof It is sufficient to prove the implication for the basis $Y_j^k, k = 1, \dots, N_{j,d}$, because of the linearity of the integral. For these

$$\int_{\mathbb{S}^{d-1}} K(\xi, \zeta) \overline{Y_j^k(\xi)} d\sigma(\xi) = \sum_{j'=0}^{\infty} \sum_{k'=1}^{N_{j',d}} a_{j,j',k,k'} Y_{j'}^{k'}(\zeta),$$

which is an element of H_j if and only if $a_{j,j',k,k'} = \delta_{j,j'} d_j(k, k')$. □

Kernels of this form, we call them convolutional kernels, are invariant under parity, meaning $K(\xi, \zeta) = K(-\xi, -\zeta)$, and the special structure allows to determine easily if an interpolant derived using such a kernel is included in certain Sobolev spaces, as for example studied in [22].

The kernels have been mostly discussed without the selection of a fixed basis of the spherical harmonics of a certain order. In this case one can choose the basis of H_j , denoted by $\tilde{Y}_j^k(\xi)$ in a way that

$$K(\xi, \zeta) = \sum_{j=0}^{\infty} \sum_{k=1}^{N_{j,d}} d_{j,k} \tilde{Y}_j^k(\xi) \overline{\tilde{Y}_j^k(\zeta)}, \quad \forall \xi, \zeta \in \mathbb{S}^{d-1}. \tag{10}$$

Under the above conditions and for $f \in L^2(\mathbb{S}^{d-1})$ the convolution operator with kernel K is

$$Tf(\xi) = \int_{\mathbb{S}^{d-1}} K(\xi, \zeta) f(\zeta) d\sigma(\zeta),$$

and the Fourier coefficients of Tf as in (6), when computed with respect to the basis \tilde{Y}_j^k , satisfy $\widehat{Tf}_{j,k} = d_{j,k} \hat{f}_{j,k}$. We nevertheless include the slightly more complex block structure, since we believe it to be helpful when we want to construct new

kernels using our results. For example we may be using the fixed basis of the spherical harmonics on the 2-sphere as mentioned.

For completeness we include the conditions on the coefficients which ensure invariance under parity. One can easily verify that all restrictions of shift-invariant, Hermitian kernels in \mathbb{R}^d to the surface of the sphere are invariant under parity.

Lemma 4 (Parity-invariance) *A kernel with property (7) satisfies,*

$$K(\xi, \zeta) = K(-\xi, -\zeta), \quad \forall \xi, \zeta \in \mathbb{S}^{d-1},$$

if and only if

$$a_{j,j',k,k'} = 0, \quad \forall j + j' \not\equiv 0 \pmod{2}. \tag{11}$$

Proof The result follows immediately using the property of homogeneity of the spherical harmonics:

$$K(-\xi, -\zeta) = \sum_{j=0}^{\infty} \sum_{k=1}^{N_{j,d}} \sum_{j'=0}^{\infty} \sum_{k'=1}^{N_{j',d}} a_{j,j',k,k'} (-1)^{j+j'} \overline{Y_{j'}^{k'}(\zeta)} Y_j^k(\xi), \quad \forall \xi, \zeta \in \mathbb{S}^{d-1}.$$

This is equal to $K(\xi, \zeta)$ if and only if all coefficients are equal, meaning $a_{j,j',k,k'} = 0$, for all pairs of j, j' with odd sum. □

The previous conditions are independent of the choice of orthogonal basis Y_j^k . For axial symmetry we will have to fix a certain basis. For the existing results for $d = 3$ this was (4) where axial symmetry with respect to φ led to the coefficients satisfying $a_{j,j',k,k'} = \delta_{k,k'} c_{j,j'}$. On general spheres with $d \geq 3$ we will focus on axial symmetry with respect to just one of the $d - 1$ axes and we assume that the sphere has been rotated such that this is the axis which is represented by the first coordinate in the polar coordinate representation of $\xi \in \mathbb{S}^{d-1}$, which we denote by $(\theta_1, \dots, \theta_{d-1})^T \in [0, 2\pi) \times [0, \pi)^{d-2}$. The spherical harmonics of degree ℓ_{d-1} can explicitly be given by

$$Y_{\ell_1, \dots, \ell_{d-1}}(\xi) = \frac{1}{\sqrt{2\pi}} e^{i\ell_1\theta_1} \prod_{j=2}^{d-1} {}_j\tilde{P}_{\ell_j}^{\ell_{j-1}}(\theta_j), \tag{12}$$

where $\ell_1, \dots, \ell_{d-1}$ are integers satisfying

$$\ell_{d-1} \geq \dots \geq |\ell_1|$$

and

$${}_j\tilde{P}_L^\ell(\theta) = {}_j c_L^\ell (\sin(\theta))^{-(2-j)/2} P_{L+(j-2)/2}^{-(\ell+(j-2)/2)}(\cos(\theta)),$$

where P_ν^μ are the associated Legendre functions and

$${}_j c_L^\ell := \left(\frac{2L + j - 1}{2} \frac{(L + \ell + j - 2)!}{(L - \ell)!} \right)^{1/2}.$$

The formula is taken from [15], Equation (2.5). To be able to handle the formula better we define the last part of the spherical harmonics as $\ell := (\ell_2, \dots, \ell_{d-2}, \ell_{d-1})$, $\theta' := (\theta_2, \dots, \theta_{d-1})$ and

$$p_{\ell_1, \ell}(\theta') = \frac{1}{\sqrt{2\pi}} \prod_{j=2}^{d-1} j \tilde{P}_{\ell_j}^{\ell_{j-1}}(\theta_j).$$

Further we set

$$\Lambda_{|\ell_1|} := \left\{ (\ell_2, \dots, \ell_{d-2}, \ell_{d-1}) \in \mathbb{N}^{d-2} \mid |\ell_1| \leq \ell_2 \leq \dots \leq \ell_{d-2} \leq \ell_{d-1} \right\}$$

and will use $Y_{\ell_1, \ell}(\xi)$, with $\ell = (\ell_2, \dots, \ell_{d-1}) \in \Lambda_{|\ell_1|}$ as the abbreviation for $Y_{\ell_1, \ell_2, \dots, \ell_{d-1}}(\xi)$, for $a_{\ell_1, \ell_2, \dots, \ell_{d-1}, \ell'_1, \dots, \ell'_{d-1}}$ respectively. As in the definition of the spherical harmonics, we need to use the points on \mathbb{S}^{d-1} and their polar coordinates simultaneously, therefore we note that ξ has the polar coordinate representation $(\theta_1, \dots, \theta_{d-1})$ and ζ is given in polar coordinates as $(\nu_1, \dots, \nu_{d-1})$. We will consistently use this notation in the paper. Assuming a kernel has property (7) for absolute summability then it can be represented as:

$$K(\xi, \zeta) = \frac{1}{2\pi} \sum_{\ell_1, \ell'_1=-\infty}^{\infty} \sum_{\ell \in \Lambda_{|\ell_1|}} \sum_{\ell' \in \Lambda_{|\ell'_1|}} a_{\ell_1, \ell, \ell'_1, \ell'} e^{i(\ell_1 \theta_1 - \ell'_1 \nu_1)} p_{\ell_1, \ell}(\theta')(\xi) \overline{p_{\ell'_1, \ell'}(\nu')(\zeta)}, \tag{13}$$

by reordering of the summands.

Theorem 1 (Axial symmetry with respect to one axis) *A kernel with property (7), given in the form*

$$K(\xi, \zeta) = \sum_{\ell_1, \ell'_1=-\infty}^{\infty} \sum_{\ell \in \Lambda_{|\ell_1|}} \sum_{\ell' \in \Lambda_{|\ell'_1|}} a_{\ell_1, \ell, \ell'_1, \ell'} Y_{\ell_1, \ell}(\xi) \overline{Y_{\ell'_1, \ell'}(\zeta)}, \quad \xi, \zeta \in \mathbb{S}^{d-1},$$

is axially symmetric with respect to the θ_1 axis if and only if

$$a_{\ell_1, \ell, \ell'_1, \ell'} = \delta_{\ell_1, \ell'_1} c_{\ell_1}(\ell, \ell'). \tag{14}$$

Proof The rotation in the θ_1 -axis by the angle α will be denoted as R_α . Then using (13):

$$\begin{aligned} K(R_\alpha \xi, R_\alpha \zeta) &= \sum_{\ell_1, \ell'_1=-\infty}^{\infty} \sum_{\ell \in \Lambda_{|\ell_1|}} \sum_{\ell' \in \Lambda_{|\ell'_1|}} a_{\ell_1, \ell, \ell'_1, \ell'} \frac{1}{2\pi} e^{i\ell_1(\theta_1+\alpha) - i\ell'_1(\nu_1+\alpha)} \\ &\quad \times p_{\ell'_1, \ell}(\theta')(\xi) \overline{p_{\ell'_1, \ell'}(\nu')(\zeta)} \\ &= \sum_{\ell_1, \ell'_1=-\infty}^{\infty} e^{-i\alpha(\ell_1 - \ell'_1)} \times \sum_{\ell \in \Lambda_{|\ell_1|}} \sum_{\ell' \in \Lambda_{|\ell'_1|}} a_{\ell_1, \ell, \ell'_1, \ell'} Y_{\ell_1, \ell}(\xi) \overline{Y_{\ell'_1, \ell'}(\zeta)}. \end{aligned} \tag{15}$$

We see that the above condition is sufficient for axial symmetry. It is also necessary since according to Lemma 1 equality is only possible if the coefficients are all equal and this can only hold for all $\alpha > 0$ if $a_{\ell_1, \ell, \ell', \ell'} = \delta_{\ell_1, \ell'} c_{\ell_1}(\ell, \ell')$. \square

As expected, the axially symmetric kernels can be written as a function depending on the values θ', v' and the longitudinal difference $\theta_1 - v_1$. In [11] additionally the properties of being longitudinal independent and longitudinal-reversible are introduced.

Definition 2 – An axially symmetric kernel is called longitudinal reversible if there exists a map $\tilde{K} : [0, 2\pi) \times [0, \pi)^{d-2} \times [0, \pi)^{d-2} \rightarrow \mathbb{C}$ with

$$K(\xi, \zeta) = \tilde{K}(|\theta_1 - v_1|, \theta', v').$$

– An axially symmetric kernel is called longitudinal-independent if there exists a map $\tilde{K} : [0, \pi)^{d-2} \times [0, \pi)^{d-2} \rightarrow \mathbb{C}$ with

$$K(\xi, \zeta) = \tilde{K}(\theta', v').$$

For the next lemma and further use in the next section we introduce another simplified notation. First we define for an axially symmetric Hermitian kernel

$$c_{\ell_1} : \Lambda_{|\ell_1|} \times \Lambda_{|\ell_1|} \rightarrow \mathbb{C}, \tag{16}$$

where the values of the map are as in (14). We deduce from Theorem 1 that every Hermitian, continuous and axially symmetric kernel which satisfies (7) can therefore be written as

$$K(\xi, \zeta) = \sum_{\ell_1=-\infty}^{\infty} \sum_{\ell, \ell' \in \Lambda_{|\ell_1|}} c_{\ell_1}(\ell, \ell') Y_{\ell_1, \ell}(\xi) \overline{Y_{\ell_1, \ell'}(\zeta)}. \tag{17}$$

Additionally, we find that these spherical harmonics can be represented as

$$Y_{\ell_1, \ell}(\xi) = \begin{cases} e^{i\ell_1\theta_1} p_{\ell_1, \ell}(\theta'), & \ell_1 \geq 0, \\ (-1)^{\ell_1} e^{i\ell_1\theta_1} p_{-\ell_1, \ell}(\theta'), & \ell_1 < 0, \end{cases} \tag{18}$$

where $\theta' = (\theta_2, \dots, \theta_{d-1})$, $p_{\ell_1, \ell}$ is real valued, and the representation follows from (12).

We briefly state sufficient conditions of the expansion coefficients for longitudinal reversibility and independence.

Lemma 5 1. *An axially symmetric kernel satisfying (7) is longitudinal reversible if and only if*

$$c_{\ell_1}(\ell, \ell') = c_{-\ell_1}(\ell, \ell'), \quad \forall \ell_1 \in \mathbb{Z}, \ell, \ell' \in \Lambda_{|\ell_1|}.$$

2. An axially symmetric kernel satisfying (7) is longitudinal independent if and only if $c_{\ell_1}(\ell, \ell') = 0$ for all $\ell_1 \neq 0$.
3. An axially symmetric kernel satisfying (7) with the above expansion is real valued if and only if

$$c_{\ell_1}(\ell, \ell') = \overline{c_{-\ell_1}(\ell, \ell')}, \quad \forall \ell_1 \in \mathbb{Z}, \ell, \ell' \in \Lambda_{|\ell_1|}. \tag{19}$$

Proof 1. Using the above representation of the spherical harmonics for ξ and ζ , we find

$$K(\xi, \zeta) = \sum_{\ell_1=-\infty}^{\infty} \sum_{\ell, \ell' \in \Lambda_{|\ell_1|}} c_{\ell_1}(\ell, \ell') e^{i\ell_1\theta_1 - i\ell_1\nu_1} p_{\ell_1, \ell}(\theta') p_{\ell_1, \ell'}(\nu').$$

If we denote by ξ' the point on \mathbb{S}^{d-1} with polar coordinates $(\nu_1, \theta_2, \dots, \theta_{d-1})$ and by ζ' the point with polar coordinates $(\theta_1, \nu_2, \dots, \nu_{d-1})$ then a kernel is longitudinal reversible if $K(\xi, \zeta) = K(\xi', \zeta')$ for all $\xi, \zeta \in \mathbb{S}^{d-1}$. It follows as above

$$\begin{aligned} K(\xi', \zeta') &= \sum_{\ell_1=-\infty}^{\infty} \sum_{\ell, \ell' \in \Lambda_{|\ell_1|}} c_{\ell_1}(\ell, \ell') e^{i(-\ell_1)(\theta_1 - \nu_1)} p_{\ell_1, \ell}(\theta') p_{\ell_1, \ell'}(\nu') \\ &= \sum_{\ell_1=-\infty}^{\infty} \sum_{\ell, \ell' \in \Lambda_{|\ell_1|}} c_{-\ell_1}(\ell, \ell') e^{i\ell_1\theta_1 - i\ell_1\nu_1} (-1)^{2\ell_1} p_{\ell_1, \ell}(\theta') p_{\ell_1, \ell'}(\nu') \\ &= \sum_{\ell_1=-\infty}^{\infty} \sum_{\ell, \ell' \in \Lambda_{|\ell_1|}} c_{-\ell_1}(\ell, \ell') Y_{\ell_1, \ell}(\xi) \overline{Y_{\ell_1, \ell'}(\zeta)}. \end{aligned}$$

The result is a consequence of the uniqueness of the series representation.

2. The sufficiency of the second part follows directly from the representation. Since

$$\begin{aligned} K(\xi, \zeta) &= \sum_{\ell_1=1}^{\infty} \sum_{\ell, \ell' \in \Lambda_{|\ell_1|}} \left(e^{i\ell_1(\theta_1 - \nu_1)} c_{\ell_1}(\ell, \ell') + (-1)^{2\ell_1} e^{-i\ell_1(\theta_1 - \nu_1)} c_{-\ell_1}(\ell, \ell') \right) \\ &\quad \times p_{\ell_1, \ell}(\theta') p_{\ell_1, \ell'}(\nu') + \sum_{\ell, \ell' \in \Lambda_0} c_0(\ell, \ell') p_{0, \ell}(\theta') p_{0, \ell'}(\nu') \end{aligned}$$

shows that if all c_{ℓ_1} are constant zero for $\ell_1 \neq 0$ the kernel is independent of the values θ_1, ν_1 . For the necessity we use that

$$K(\xi, \zeta) = \sum_{\ell_1=-\infty}^{\infty} e^{i\ell_1(\theta_1 - \varphi_1)} \sum_{\ell, \ell' \in \Lambda_{|\ell_1|}} c_{\ell_1}(\ell, \ell') p_{\ell_1, \ell}(\theta') p_{\ell_1, \ell'}(\varphi')$$

is constant as a function of $(\theta_1 - \varphi_1) \in (-2\pi, 2\pi)$ if and only if the second sum is zero for all $\ell_1 \neq 0$ and θ', φ' .

3. We use the same representation above for the kernels $K(\xi, \zeta)$ as well as for its complex conjugate:

$$\begin{aligned} \overline{K(\xi, \zeta)} &= \sum_{\ell_1=-\infty}^{\infty} e^{-i\ell_1(\theta_1-\nu_1)} \sum_{\ell, \ell' \in \Lambda_{|\ell_1|}} \overline{c_{\ell_1}(\ell, \ell')} p_{\ell_1, \ell}(\theta') p_{\ell_1, \ell'}(\nu') \\ &= \sum_{\ell_1=-\infty}^{\infty} e^{i(-\ell_1)(\theta_1-\nu_1)} \sum_{\ell, \ell' \in \Lambda_{|\ell_1|}} \overline{c_{\ell_1}(\ell, \ell')} (-1)^{2\ell_1} p_{-\ell_1, \ell}(\theta') p_{-\ell_1, \ell'}(\nu') \end{aligned}$$

and deduce that because of the uniqueness of the expansion coefficients, the two are equal if and only if $\overline{c_{\ell_1}(\ell, \ell')} = c_{-\ell_1}(\ell, \ell')$ for all $\ell_1 \in \mathbb{Z}$ and $\ell, \ell' \in \Lambda_{|\ell_1|}$. \square

We note that in distinction to the results for invariance under parity and convolutional form the given results on axially-symmetric kernels are basis dependent. For example using a real basis of the spherical harmonics would change condition (19) to the coefficient having to be real. We finally summarise the connections between the introduced properties, which follows directly from the definitions.

Lemma 6 *We assume the kernels in this proposition to be Hermitian and to satisfy (7).*

1. *In the case $d = 2$ all axially symmetric kernels have convolutional form.*
2. *An axially symmetric kernel given in the form Eq. (17) has a convolutional form if and only if*

$$c_{\ell_1}(\ell_2, \dots, \ell_{d-1}, \ell'_2, \dots, \ell'_{d-1}) = 0$$

for all $\ell_{d-1} \neq \ell'_{d-1} \in \mathbb{N}_0$.

3 (Strict) Positive Definiteness of Axially Symmetric Kernels

In [6] strictly positive definite axially symmetric kernels on the 2-sphere were described and sufficient conditions for strict positive definiteness stated. We add sufficient conditions for d -dimensional spheres and prove some additional necessary conditions. In this section we focus on kernels on spheres with $d \geq 3$, the special case of the circle is discussed in Section 5.

From now on we will use property (7) also for axially symmetric and convolutional kernels. In this case the coefficients $a_{j, j', k, k'}$ in (7) are derived using (16) and (14) for axially symmetric kernels and (9) in the convolutional case.

Theorem 2 *Let K be a Hermitian, axially symmetric kernel with property (7) given in the form (17), with $d \geq 3$. The kernel is positive definite if and only if the mapping $c_{\ell_1} : \Lambda_{|\ell_1|} \times \Lambda_{|\ell_1|} \rightarrow \mathbb{C}$ is positive definite for all $\ell_1 \in \mathbb{Z}$.*

Proof For the first direction we rewrite the quadratic form

$$\sum_{\xi, \zeta \in \Xi} \lambda_{\xi} \overline{\lambda_{\zeta}} K(\xi, \zeta) = \sum_{\ell_1=-\infty}^{\infty} \sum_{\ell, \ell' \in \Lambda_{|\ell_1|}} c_{\ell_1}(\ell, \ell') \sum_{\xi \in \Xi} \lambda_{\xi} Y_{\ell_1, \ell}(\xi) \overline{\sum_{\zeta \in \Xi} \lambda_{\zeta} Y_{\ell_1, \ell'}(\zeta)}.$$

Now we define $\underline{\ell} = (\ell_2, \dots, \ell_{d-2})$, $y_{\underline{\xi}}^{\ell_1, \underline{\ell}, \ell_{d-1}} := \sum_{\xi \in \mathbb{S}} \lambda_{\xi} Y_{\ell_1, \underline{\ell}, \ell_{d-1}}(\xi) \in \mathbb{C}$ to find

$$\sum_{\xi, \zeta \in \mathbb{S}} \lambda_{\xi} \overline{\lambda_{\zeta}} K(\xi, \zeta) = \sum_{\ell_1 = -\infty}^{\infty} \lim_{k \rightarrow \infty} \sum_{\ell_{d-1}, \ell'_{d-1} = |\ell_1|}^k \sum_{\underline{\ell} \in \Lambda_{\ell_1, \ell_{d-1}}} \sum_{\underline{\ell}' \in \Lambda_{\ell_1, \ell'_{d-1}}} y_{\underline{\xi}}^{\ell_1, \underline{\ell}, \ell_{d-1}} c_{\ell_1}((\underline{\ell}, \ell_{d-1}), (\underline{\ell}', \ell'_{d-1})) \overline{y_{\underline{\xi}}^{\ell_1, \underline{\ell}', \ell'_{d-1}}},$$

where

$$\Lambda_{\ell_1, \ell_{d-1}} := \left\{ (\ell_2, \dots, \ell_{d-2}) \in \mathbb{N}_0^{d-3} \mid |\ell_1| \leq \ell_2 \leq \dots \leq \ell_{d-2} \leq \ell_{d-1} \right\}$$

and the absolute summability ensures equality after reordering. The positive definiteness of the mapping c_{ℓ_1} implies that

$$\sum_{\ell_{d-1}, \ell'_{d-1} = |\ell_1|}^k \sum_{\underline{\ell} \in \Lambda_{\ell_1, \ell_{d-1}}} \sum_{\underline{\ell}' \in \Lambda_{\ell_1, \ell'_{d-1}}} d_{\underline{\ell}, \ell_{d-1}} c_{\ell_1}((\underline{\ell}, \ell_{d-1}), (\underline{\ell}', \ell'_{d-1})) \overline{d_{\underline{\ell}', \ell'_{d-1}}} \geq 0,$$

for all $\ell_1 \in \mathbb{Z}$, $k \geq |\ell_1|$ and arbitrary values $d_{\underline{\ell}, \ell_{d-1}} \in \mathbb{C}$. Thereby the limit in the penultimate equation is non-negative for all ℓ_1 and thereby the infinite sum is as well.

The necessity of the positive definiteness of the c_{ℓ_1} is proven by contradiction. If we assume there exists an $\ell_1 \in \mathbb{Z}$, a finite set $\Lambda \subset \Lambda_{\ell_1}$ and coefficients $d_{\ell} \in \mathbb{C}$ for $\ell \in \Lambda$ satisfying

$$\sum_{\ell, \ell' \in \Lambda} d_{\ell} c_{\ell_1}(\ell, \ell') \overline{d_{\ell'}} < 0$$

then we can define $f(\xi) = \sum_{\ell \in \Lambda} d_{\ell} Y_{\ell_1, \ell}(\xi) \in C(\mathbb{S}^{d-1})$ and deduce

$$\int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} f(\xi) K(\xi, \zeta) \overline{f(\zeta)} d\xi d\zeta < 0.$$

This contradicts the positive definiteness of K since the equivalence of positive definiteness and integral positive definiteness has been established for general Riemannian manifolds in Theorem 2.1 in [9]. □

We do not need the property of positive definiteness for arbitrary values of the index set in the proof of the result. Therefore we can loosen the assumption by introducing a matrix-like notation for the mapping. We first introduce a new index α where $\alpha \in \mathbb{N}$ and there is a one-to one mapping from \mathbb{N} to the pairs

$$(\underline{\ell}_{\alpha}, \ell_{d-1, \alpha}) \in \Lambda_{|\ell_1|}$$

satisfying $\ell_{d-1, \alpha'} \leq \ell_{d-1, \alpha}$ if $\alpha' < \alpha$. For the proof, the actual order of the mapping is insignificant. We additionally define for each α the eigenvalue corresponding to $Y_{\ell_1, \underline{\ell}_{\alpha}, \ell_{d-1, \alpha}}$ by λ_{α} which only depends on the value of $\ell_{d-1, \alpha}$. Further we introduce

the notation $N_\alpha := N_{\ell_{d-1}, \alpha, d}$ for the number of spherical harmonics corresponding to the eigenvalue λ_α .

Then we define for each $k \in \mathbb{N}$:

$$A_{\ell_1}^k = (c_{\ell_1}(\underline{\ell}_\alpha, \ell_{d-1}, \alpha, \underline{\ell}_{\alpha'}, \ell_{d-1}, \alpha'))_{\alpha, \alpha'=1}^k. \tag{20}$$

We note that in the case of $d = 3$ the matrix structure of the mappings c_{ℓ_1} is evident since $A_{|\ell_1|} = \{j \in \mathbb{N}_0 \mid j \geq |\ell_1|\}$.

Proposition 1 *Let K be a Hermitian, axially symmetric kernel of the form (17), $d \geq 3$, with property (7) and $A_{\ell_1}^k$ as above. The kernel is positive definite if and only if the matrix $A_{\ell_1}^k$ is positive semi-definite for all $\ell_1 \in \mathbb{Z}$ and all $k \in \mathbb{N}$.*

The proof is similar to the proof of Theorem 2 and therefore omitted.

For the investigation of strict positive definiteness of axially symmetric kernels we present two approaches. For the first we continue to use the matrix representation introduced in the last proposition and for the second we will be using the mappings c_{ℓ_1} and sets of indices $\ell_1 \in \mathbb{Z}$ which also allow to deduce strict positive definiteness.

Lemma 7 *For K as in the above proposition. The kernel is strictly positive definite if and only if for each $\ell_1 \in \mathbb{N}$ there exist a sequence with positive entries $d_j^{\ell_1} > 0$, $j \in \mathbb{N}$, such that the matrix*

$$\tilde{A}_{\ell_1}^k = D_k^{1/2} A_{\ell_1}^k D_k^{1/2}, \quad \text{with } D_k = \left(\delta_{i,j} d_j^{\ell_1} \right)_{i,j=1}^k$$

satisfies

$$\lambda_{\min} \left(\tilde{A}_{\ell_1}^k \right) > \varepsilon_{\ell_1},$$

where $\varepsilon_{\ell_1} > 0$ is independent of k .

Proof From the proof of the last lemma we deduce:

$$\sum_{\xi, \zeta \in \mathcal{E}} \lambda_\xi \overline{\lambda_\zeta} K(\xi, \zeta) = \sum_{\ell_1=-\infty}^{\infty} \lim_{k \rightarrow \infty} \left(\mathbf{y}^{\ell_1, k} \right)^T A_{\ell_1}^k \overline{\mathbf{y}^{\ell_1, k}}$$

where $\mathbf{y}^{\ell_1, k} = \left(y_{\underline{\mathcal{E}}}^{\ell_1, \underline{\ell}_\alpha, \ell_{d-1}, \alpha} \right)_{\alpha=1}^k$.

Now we employ the definition of $\tilde{A}_{\ell_1}^k$ in order to find

$$\begin{aligned} \sum_{\xi, \zeta \in \mathcal{E}} \lambda_\xi \overline{\lambda_\zeta} K(\xi, \zeta) &= \sum_{\ell_1=-\infty}^{\infty} \lim_{k \rightarrow \infty} \left(\mathbf{y}^{\ell_1, k} \right)^T D_k^{-1/2} \tilde{A}_{\ell_1}^k D_k^{-1/2} \overline{\mathbf{y}^{\ell_1, k}} \\ &\geq \sum_{\ell_1=-\infty}^{\infty} \lim_{k \rightarrow \infty} \| D_k^{-1/2} \mathbf{y}^{\ell_1, k} \|_2^2 \lambda_{\min} \left(\tilde{A}_{\ell_1}^k \right) \\ &> \sum_{\ell_1=-\infty}^{\infty} \lim_{k \rightarrow \infty} \varepsilon_{\ell_1} \left(\| D_k^{-1/2} \mathbf{y}^{\ell_1, k} \|_2 \right)^2, \end{aligned}$$

where in the second line we use that $\tilde{A}_{\ell_1}^k$ is positive definite because its smallest eigenvalue is strictly positive.

Thereby

$$\begin{aligned} \sum_{\xi \in \mathcal{E}} \sum_{\zeta \in \mathcal{E}} \lambda_\xi \bar{\lambda}_\zeta K(\xi, \zeta) &> \sum_{\ell_1=-\infty}^{\infty} \varepsilon_{\ell_1} \lim_{k \rightarrow \infty} \left\| \left(D_k^{-1/2} \mathbf{y}^{\ell_1, k} \right) \right\|_2^2 \\ &\geq \sum_{\ell_1=-\infty}^{\infty} \varepsilon_{\ell_1} \sum_{\alpha=1}^{\infty} \left(\left(d_\alpha^{\ell_1} \right)^{-1/2} \left| y_{\mathcal{E}}^{\ell_1, \ell_\alpha, \ell_{d-1, \alpha}} \right|^2 \right), \end{aligned}$$

where the last sum can only be zero if $y_{\mathcal{E}}^{\ell_1, \ell_\alpha, \ell_{d-1, \alpha}}$ is a zero sequence for all ℓ_1 . This implies that the λ_ξ in the definition of the quadratic form need all be zero as a consequence of the linear independence of the spherical harmonics. \square

We give a simple example of kernels for which strict positive definiteness can be proven using the above result. Let the kernel take the form:

$$K(\xi, \zeta) = \sum_{\ell_1=-\infty}^{\infty} \sum_{\ell \in \Lambda_{|\ell_1|}} c_{\ell_1}(\ell, \ell) Y_{\ell_1, \ell}(\xi) \overline{Y_{\ell_1, \ell}(\zeta)},$$

where $c_{\ell_1}(\ell, \ell) > 0$ and satisfies condition (7). Then $A_{\ell_1}^k$ is a diagonal matrix with positive entries. Setting $D_k = (\delta_{i,j} c_{\ell_1}(i, i))_{i,j=1}^{\infty}$ results in $\tilde{A}_{\ell_1}^k = I$ and thereby the resulting kernel will be strictly positive definite. The described kernels are not isotropic but have convolutional form and therefore we will be able to give a more general condition in the next section.

Theorem 3 *Let K be a Hermitian, axially symmetric kernel of the form (17) satisfying (7) for absolute summability and $d > 2$. The kernel is strictly positive definite if*

$$\tilde{A}_{\ell_1} = \left(\tilde{a}_{\alpha, \alpha'}^{\ell_1} \right)_{\alpha, \alpha'=1}^{\infty} = \left(\sqrt{N_\alpha} c_{\ell_1}(\underline{\ell}_\alpha, \ell_{d-1, \alpha}, \underline{\ell}_{\alpha'}, \ell_{d-1, \alpha'}) \sqrt{N_{\alpha'}} \right)_{\alpha, \alpha'=1}^{\infty}$$

is positive definite on $\ell^\infty(\mathbb{N})$ for all $\ell_1 \in \mathbb{N}$ and satisfies the uniform strict diagonal dominance property:

$$\sum_{\alpha' \neq \alpha} |\tilde{a}_{\alpha, \alpha'}^{\ell_1}| < \sigma_{\ell_1} |\tilde{a}_{\alpha, \alpha}^{\ell_1}|, \quad \forall \alpha \in \mathbb{N},$$

where each $0 < \sigma_{\ell_1} < 1$ is independent of α .

Proof We denote by $\tilde{A}_{\ell_1} = G_{\ell_1} G_{\ell_1}^*$ the infinite Cholesky decomposition matrix which exists since \tilde{A}_{ℓ_1} is positive definite and bounded on $\ell^\infty(\mathbb{N})$ as a consequence of (7).

Inserting the Cholesky-decomposition into the quadratic form

$$\sum_{\xi \in \mathcal{E}} \sum_{\zeta \in \mathcal{E}} \lambda_\xi \bar{\lambda}_\zeta K(\xi, \zeta) = \sum_{\ell_1=-\infty}^{\infty} \left\| G_{\ell_1}(\tilde{\mathbf{y}}^{\ell_1}) \right\|_2^2, \tag{21}$$

where $\tilde{\mathbf{y}}^{\ell_1} = \left(\frac{1}{\sqrt{N_\alpha}} y_{\mathcal{E}}^{\ell_1, \ell_\alpha, \ell_{d-1}, \alpha}\right)_{\alpha=1}^\infty$ is a bounded sequence as a result of the estimate of the spherical harmonics in (5). We first deduce that if there exists an element of the space of bounded sequences $\ell^\infty(\mathbb{N})$ for which $G_{\ell_1}^* x = 0$, then $G_{\ell_1} \left(G_{\ell_1}^* x\right) = \tilde{A}_{\ell_1} x = 0$, where we can exchange the order of multiplication because of the triangular structure of G_{ℓ_1} and because $G_{\ell_1}^* x$ is elementwise finite for all bounded x . This is a result of $\|G_{\ell_1}^* x\|^2 = \bar{x}^T \tilde{A}_{\ell_1} x < \infty$ which follows from (7).

Thereby it is sufficient to show that there exists no eigenvector in the space of bounded sequences for which $\tilde{A}_{\ell_1} x = 0$. We prove this by contradiction, adapting the conditions of [27] Theorem 1b.

From the positive definiteness of the sub-matrices of \tilde{A}^{ℓ_1} we can deduce that $\tilde{a}_{\alpha, \alpha}^{\ell_1}$ is non-zero for all $\alpha \in \mathbb{N}$. Thereby

$$\begin{aligned} &\sum_{\alpha'=0}^\infty \tilde{a}_{\alpha, \alpha'}^{\ell_1} x_{\alpha'} = 0, \quad \forall \alpha \in \mathbb{N}_0, \\ \Leftrightarrow &\sum_{\alpha' \neq \alpha} \tilde{a}_{\alpha, \alpha'}^{\ell_1} x_{\alpha'} = -\tilde{a}_{\alpha, \alpha}^{\ell_1} x_\alpha, \quad \forall \alpha \in \mathbb{N}_0. \end{aligned}$$

Since x has ℓ^∞ -norm one, there exists a value $\alpha \in \mathbb{N}_0$, for which $|x_\alpha| > \sigma_{\ell_1}$ and

$$\sum_{\alpha' \neq \alpha} |\tilde{a}_{\alpha, \alpha'}^{\ell_1}| \geq \sum_{\alpha' \neq \alpha} |\tilde{a}_{\alpha, \alpha'}^{\ell_1} x_{\alpha'}| \geq |\tilde{a}_{\alpha, \alpha}^{\ell_1}| \sigma_{\ell_1}.$$

This contradicts the assumption and the only possible choice for which (21) is equal to zero is $\tilde{\mathbf{y}}^{\ell_1} = 0$ for all $\ell_1 \in \mathbb{Z}$. From the definition of this sequence we know that this is only possible if $\lambda_\xi = 0$ for all $\xi \in \mathcal{E}$ as in the proof of the last lemma. \square

Examples for kernels for which this result is applicable are all kernels where a certain ordering of the coefficients leads to A_{ℓ_1} having the form of a general band matrix.

We wish to find more general sufficient conditions that are easy to evaluate. They will be stronger than simply demanding that c_{ℓ_1} be strictly positive definite, which would only allow a finite subset of the indices Λ_{ℓ_1} to be used in a quadratic form.

Therefore we define the set \mathcal{F} as the set of all indices $\ell_1 \in \mathbb{Z}$ for which

$$\text{there exists } j \in \Lambda_{|\ell_1|}, d_j \neq 0 \Rightarrow \sum_{j, j' \in \Lambda_{|\ell_1|}} d_j c_{\ell_1}(j, j') \bar{d}_{j'}$$

does not converge to zero.

Lemma 8 *A Hermitian axially symmetric kernel K of the form (17), satisfying (7), with positive definite maps $c_{\ell_1} : \Lambda_{|\ell_1|} \times \Lambda_{|\ell_1|} \rightarrow \mathbb{C}$ is strictly positive definite if*

$$\sum_{\xi \in \mathcal{E}} \lambda_\xi Y_{\ell_1, \ell}(\xi) = 0 \quad \forall \ell_1 \in \mathcal{F}, \ell \in \Lambda_{|\ell_1|} \Rightarrow \lambda_\xi = 0 \quad \forall \xi \in \mathcal{E}.$$

Proof We prove the result by contradiction and assume that K is positive definite but not strictly positive definite. If K is not strictly positive definite there exists a nonempty set of distinct points \mathcal{E} and coefficients λ_ξ not all zero with

$$\sum_{\xi, \zeta \in \mathcal{E}} \lambda_\xi \overline{\lambda_\zeta} K(\xi, \zeta) = 0.$$

This is equivalent according to the computation in the proof of Theorem 2 to

$$\sum_{\ell_1 = -\infty}^{\infty} \sum_{\ell, \ell' \in \Lambda_{|\ell_1|}} c_{\ell_1}(\ell, \ell') Y_{\ell_1, \ell, \mathcal{E}} \overline{Y_{\ell_1, \ell', \mathcal{E}}} = 0, \tag{22}$$

where $Y_{\ell_1, \ell, \mathcal{E}} = \sum_{\xi \in \mathcal{E}} \lambda_\xi Y_{\ell_1, \ell}(\xi)$.

Since we know that all the sums are non-negative because the maps c_{ℓ_1} are all positive definite, the overall sum can only be zero if all summands are. For the indices $\ell_1 \in \mathcal{F}$ this implies $Y_{\ell_1, \ell, \mathcal{E}} = 0$, because the convergence of the sum is ensured by property (7). But according to the condition of the lemma this implies $\lambda_\xi = 0$ for all $\xi \in \mathcal{E}$, in contradiction to the assumption of the proof. \square

With the goal of understanding which sets \mathcal{F} lead to strictly positive definite kernels we first state a simple sufficient condition. The following proposition is an immediate consequence of the last lemma together with the linear independence of the spherical harmonics.

Proposition 2 *A kernel as in in the last lemma is strictly positive definite if $\mathcal{F} = \mathbb{Z}$.*

For the special case $d = 3$, this result was proven in [6] as Theorem 2, where the assumptions on the maps can be simplified because of the specific structure of \mathbb{S}^2 . As a next step we study necessary conditions:

Lemma 9 *Let K be a Hermitian, axially symmetric kernel of the form (17), satisfying (7). For the kernel to be strictly positive definite it is necessary that the mapping*

$$c_{\ell_1} : \Lambda_{|\ell_1|} \times \Lambda_{|\ell_1|} \rightarrow \mathbb{C}$$

is not identically zero for infinitely many $\ell_1 \in \mathbb{Z}$.

Proof The result is proven by contradiction. Assume there are only finitely many values of ℓ_1 for which c_{ℓ_1} is not the zero mapping. Let us denote the set of these ℓ_1 by \mathcal{J} . Then we can construct a set of points \mathcal{E} and coefficients $\lambda_\xi \in \mathbb{R}$ such that

$$\sum_{\xi \in \mathcal{E}} \lambda_\xi Y_{\ell_1, \ell}(\xi) = 0, \quad \forall \ell_1 \in \mathcal{J}, \ell \in \Lambda_{|\ell_1|}. \tag{23}$$

These are infinitely many conditions since $\Lambda_{|\ell_1|}$ includes infinitely many elements but if we choose all points in \mathcal{E} of the form $(\theta_{1,k}, \theta_2, \dots, \theta_{d-1})$ for $k = 0, \dots, |\mathcal{J}|$, the above equations can be transformed into

$$\frac{1}{\sqrt{2\pi}} \prod_{j=2}^{d-1} \tilde{P}_{\ell_j}^{\ell_{j-1}}(\theta_j) \sum_{k=0}^{|\mathcal{J}|} \lambda_k e^{i\ell_1 \theta_{1,k}} = 0, \quad \forall \ell_1 \in \mathcal{J}, \ell \in \Lambda_{|\ell_1|}, \tag{24}$$

which is satisfied if

$$\sum_{k=0}^{|\mathcal{J}|} \lambda_k e^{i\ell_1 \theta_{1,k}} = 0, \quad \forall \ell_1 \in \mathcal{J}. \tag{25}$$

These are only $|\mathcal{J}|$ conditions which can be satisfied for our choice of $\theta_{1,k}$ at $|\mathcal{J}| + 1$ distinct points. □

The next result is especially interesting because for spherical radial basis functions we were used to be able to leave out finitely many indices of similar sets without loosing strict positive definiteness. This is not the case for axially symmetric kernels, where $\ell_1 = 0$ is of special importance.

Lemma 10 *Let K be a Hermitian, axially symmetric kernel of the form (17) satisfying (7). For the kernel to be strictly positive definite, it is necessary that the mapping*

$$c_0 : \Lambda_{|\ell_1|} \times \Lambda_{|\ell_1|} \rightarrow \mathbb{C}$$

is not identically zero.

Proof We show that for any point on the surface of the sphere ξ which has polar coordinates $(\theta_1, 0, \theta_3, \dots, \theta_{d-1})$, the spherical basis functions $Y_{\ell_1, \ell}(\xi)$ only take non-zero values if $\ell_1 = 0$. Inserting the point into the definition of the spherical harmonics from (12)

$$\begin{aligned} Y_{\ell_1, \ell}(\xi) &= \frac{1}{\sqrt{2\pi}} e^{i\ell_1 \theta_1} \prod_{j=2}^{d-1} \tilde{P}_{\ell_j}^{\ell_{j-1}}(\theta_j) \\ &= \frac{1}{\sqrt{2\pi}} e^{i\ell_1 \theta_1} \left(\frac{2\ell_2 + 1}{2} \frac{(\ell_2 + \ell_1)!}{(\ell_2 - \ell_1)!} \right)^{1/2} P_{\ell_2}^{-\ell_1}(1) \prod_{j=3}^{d-1} \tilde{P}_{\ell_j}^{\ell_{j-1}}(\theta_j). \end{aligned}$$

Since the last part of the product is finite, the value is non-zero only if $P_{\ell_2}^{-\ell_1}(1)$ is non-zero and this is only the case for $\ell_1 = 0$. □

Two ways to construct axially symmetric kernels on the two-sphere for which the described conditions can be applied are described in [2] where the definition is via sequences and [11] via integration of isotopic kernels over arches.

4 (Strict) Positive Definiteness of Convolutional Kernels or Kernels with Eigenvalue Block Structure

We now assume that K is continuous Hermitian and has the form

$$K(\xi, \zeta) = \sum_{j=0}^{\infty} \sum_{k=1}^{N_{j,d}} \sum_{k'=1}^{N_{j,d}} d_j(k, k') Y_j^k(\xi) \overline{Y_j^{k'}(\zeta)}, \quad \forall \xi, \zeta \in \mathbb{S}^{d-1}, \quad (26)$$

for a fixed set of orthogonal basis functions, where Y_j^k is an eigenfunction corresponding to the eigenvalue λ_j of Sect. 1.1. We note that under this assumption there exists another orthonormal basis of the eigenfunctions corresponding to each eigenvalue such that, if we express K with respect to this sequence (which is also the Hilbert-Schmidt basis of the kernel), it takes the form (10). Further we emphasize that in this section we use continuity as a criterion instead of property (7), because it is the weaker assumption on the kernel.

These kernels were studied under the name convolutional kernels for example in [21, 22]. The fixed basis case on the 2-sphere was also studied in [7] and we now generalise the results.

It is proven in [10] that a continuous and Hermitian kernel K of the form (10) is positive definite if and only if the $d_{j,k}$ are real and non-negative for all $j \in \mathbb{Z}_+$, $k \in \{1, \dots, N_{j,d}\}$, (their Theorem 2.1).

We can now transfer the result known for radial kernels which was first proven in [8], to this kernel class. Since positive definiteness is independent of the choice of the expansion basis, the proofs will be carried out using kernels of the form (10) and we later briefly note the implications for fixed basis.

Lemma 11 *If a continuous and Hermitian kernel K of the form (10) is strictly positive definite, all $d_{j,k}$ are non-negative and the sequences $(d_{j,k})_{k=1}^{N_{j,d}}$ are not identically zero for infinitely many even and infinitely many odd values of $j \in \mathbb{Z}_+$.*

Proof We assume K is continuous, Hermitian and strictly positive definite. Since strict positive definiteness implies positive definiteness, the $d_{j,k}$ are all non-negative according to [10, Theorem 2]. The rest of the proof is divided into four cases. Let us denote the set of indices for which $(d_{j,k})_{k=1}^{N_{j,d}}$ are not all zero with

$$\mathcal{J} := \left\{ j \in \mathbb{Z}_+ \mid (d_{j,1}, \dots, d_{j,N_{j,d}})^T \neq \mathbf{0}^{N_{j,d}} \right\}.$$

For all four cases we assume that K is strictly positive definite of the form (10) and prove that assuming either

1. $\mathcal{J} \subset 2\mathbb{N}$ or
2. $\mathcal{J} \subset 2\mathbb{N} + 1$ or
3. $1 \leq |\mathcal{J} \cap 2\mathbb{N}| < \infty$ or
4. $1 \leq |\mathcal{J} \cap (2\mathbb{N} + 1)| < \infty$,

leads to a contradiction.

- Let us now assume $(d_{j,k})_{k=1}^{N_{j,d}}$ are not all zero *only for even* values of j . We can represent the quadratic form as

$$\begin{aligned} \sum_{\xi, \zeta \in \mathcal{E}} \lambda_\xi \overline{\lambda_\zeta} K(\xi, \zeta) &= \sum_{j=0}^{\infty} \sum_{k=1}^{N_{j,d}} d_{j,k} \sum_{\xi \in \mathcal{E}} \lambda_\xi \tilde{Y}_j^k(\xi) \overline{\sum_{\zeta \in \mathcal{E}} \lambda_\zeta \tilde{Y}_j^k(\zeta)} \\ &= \sum_{j=0}^{\infty} \sum_{k=1}^{N_{j,d}} y_{\mathcal{E}}^{j,k} d_{j,k} \overline{y_{\mathcal{E}}^{j,k}}, \quad \text{with } y_{\mathcal{E}}^{j,k} = \sum_{\xi \in \mathcal{E}} \lambda_\xi \tilde{Y}_j^k(\xi) \in \mathbb{C}. \end{aligned}$$

Choosing a non-empty set of data sites \mathcal{E}' which satisfies

$$\xi \in \mathcal{E}' \Rightarrow -\xi \in \mathcal{E}',$$

where $-\xi$ is the antipodal point of ξ , and setting $\lambda_\xi = -\lambda_{-\xi}$, we find that $y_{\mathcal{E}'}^{j,k} = 0$ for all even j since $\tilde{Y}_j^k(-\xi) = (-1)^j \tilde{Y}_j^k(\xi)$ follows from the \tilde{Y}_j^k all being homogeneous polynomials of order j . This implies $\sum_{\xi, \zeta \in \mathcal{E}'} \lambda_\xi \overline{\lambda_\zeta} K(\xi, \zeta) = 0$ and therefore K would not be strictly positive definite.

- The same argument applies when we assume $(d_{j,k})_{k=1}^{N_{j,d}}$ are not all zero *only for odd* values of j . The same set \mathcal{E}' can be chosen but now $\lambda_\xi = \lambda_{-\xi}$ yields the contradiction to the assumption of strict positive definiteness.
- Now we assume that $(d_{j,k})_{k=1}^{N_{j,d}}$ are not all zero for any number of odd values of j and *only finitely many even* values of j . Set \hat{j} to the maximal even index for which $(d_{j,k})_{k=1}^{N_{j,d}}$ is not zero. We aim to construct a set \mathcal{E} with elements only in the lower hemisphere of \mathbb{S}^{d-1} and $\lambda \in \mathbb{C}^{|\mathcal{E}|} \neq 0$, s.t. $\sum_{\xi \in \mathcal{E}} \lambda_\xi \tilde{Y}_j^k(\xi) = 0$ for all even $j \leq \hat{j}$. These are

$$M := \sum_{m=1}^{\hat{j}/2} N_{2m,d} < \infty$$

linear equations. We can therefore choose any set of distinct points in the lower hemisphere with more than M elements to find a non-trivial solution. Defining the set $\mathcal{E}' = \mathcal{E} \cup (-\mathcal{E})$ and setting $\lambda_\xi = \lambda_{-\xi}$ shows that

$$\sum_{\xi, \zeta \in \mathcal{E}'} \lambda_\xi \overline{\lambda_\zeta} K(\xi, \zeta) = 0$$

for a non-trivial vector λ and therefore K is not strictly positive definite.

- The same arguments can be used to show that $(d_{j,k})_{k=1}^{N_{j,d}}$ needs to be *non-zero for infinitely many odd* values of j .

□

For the fixed basis form this implies that for a strictly positive definite kernel of the form (26) it is necessary that the matrices $D_j := (d_j(k, k'))_{k, k'=1}^{N_{j,d}}$ are all positive

definite and infinitely many with odd j and infinitely many with even j are not the zero matrix.

With the aim of finding sufficient conditions that are easy to evaluate we define the set \mathcal{F} as the set of all indices $j \in \mathbb{Z}_+$ for which D_j is a positive definite matrix, or if the appropriate basis is used, all $d_{j,k} > 0$ for all $k = 1, \dots, N_{j,d}$.

Lemma 12 *A continuous and Hermitian kernel K of the form (26) which is positive definite is strictly positive definite if*

$$\sum_{\xi \in \mathcal{E}} \lambda_\xi Y_j^k(\xi) = 0, \forall k = 1, \dots, N_{j,d}, j \in \mathcal{F} \Rightarrow \lambda_\xi = 0, \forall \xi \in \mathcal{E}.$$

The proof follows in the same line of argument as Lemma 8.

With Lemma 12, we have shown that strict positive definiteness of these kernels can be proven using the same results which were used for zonal kernels by Chen et al. in [8] and the alternative proof for more general manifolds stated by Barbosa and Menegatto in [4]. The next lemma and Theorem 4, generalise the results to the convolutional case and complex kernels.

Lemma 13 *For a given set \mathcal{F} the following two properties are equivalent:*

1. $\sum_{\xi \in \mathcal{E}} \lambda_\xi Y_j^k(\xi) = 0, \forall k = 1, \dots, N_{j,d}, j \in \mathcal{F}$ implies $\lambda_\xi = 0, \forall \xi \in \mathcal{E}$.
2. $\sum_{\xi \in \mathcal{E}} \lambda_\xi P_j^d(\xi^T \zeta) = 0, \forall j \in \mathcal{F}, \forall \zeta \in \mathbb{S}^{d-1}$ implies $\lambda_\xi = 0, \forall \xi \in \mathcal{E}$.

Here P_j^d are the Legendre polynomials of degree j in d dimensions.

Proof Using the addition formula of the spherical harmonics we find

$$\frac{N_{j,d}}{\sigma_{d-1}} P_j^d(\xi^T \zeta) = \sum_{k=1}^{N_{j,d}} Y_j^k(\xi) \overline{Y_j^k(\zeta)}.$$

Therefore

$$\frac{N_{j,d}}{\sigma_{d-1}} \sum_{\xi \in \mathcal{E}} \lambda_\xi P_j^d(\xi^T \zeta) = \sum_{k=1}^{N_{j,d}} \left(\sum_{\xi \in \mathcal{E}} \lambda_\xi Y_j^k(\xi) \right) \overline{Y_j^k(\zeta)}, \quad \forall \zeta \in \mathbb{S}^{d-1}.$$

Since the spherical harmonics are linearly independent, the last expression is zero if and only if

$$\sum_{\xi \in \mathcal{E}} \lambda_\xi Y_j^k(\xi) = 0$$

for all $k = 1, \dots, N_{j,d}$, and all $j \in \mathcal{F}$. □

Theorem 4 *Let K be a continuous positive definite kernel of the form (26), $d > 2$, and \mathcal{F} the corresponding index set for which the D_j are positive definite matrices. Then it is sufficient for K to be strictly positive definite that \mathcal{F} includes infinitely many even and infinitely many odd values of $j \in \mathbb{Z}_+$.*

Proof Combining Lemmas 12 and 13 we know that for K to be strictly positive definite it is sufficient to prove that for arbitrary sets of distinct data sites $\mathcal{E} \subset \mathbb{S}^{d-1}$ the functions $P_j^d(\xi^T \zeta)$ satisfy Lemma 13 (2). Therefore we show that for any such set \mathcal{E}

$$\sum_{\xi \in \mathcal{E}} \lambda_\xi P_j^d(\xi^T \zeta) = 0, \quad \forall j \in \mathcal{F}, \zeta \in \mathbb{S}^{d-1},$$

implies $\lambda_\xi = 0$ for all $\xi \in \mathcal{E}$. We do this by choosing for each $\xi \in \mathcal{E}$ a corresponding $\zeta = \zeta_\xi \in \mathbb{S}^{d-1}$ and show that for this choice $\lambda_\xi = 0$ if the above holds. Assume we have fixed $\xi \in \mathcal{E}$, we need to distinguish two cases.

Case 1 $\xi^T \zeta \neq -1$ for all $\zeta \in \mathcal{E}$.

In this case we choose $\zeta_\xi = \xi$ and the system above takes the form

$$\lambda_\xi P_j^d(1) + \sum_{\zeta \in \mathcal{E} \setminus \{\xi\}} \lambda_\zeta P_j^d(\zeta^T \xi) = 0, \quad \forall j \in \mathcal{F}.$$

Note that $\xi^T \zeta \in (-1, 1)$. Since there are infinitely many indices in \mathcal{F} we can choose a sequence from \mathcal{F} with $j_n \in \mathcal{F}$ and $\lim_{n \rightarrow \infty} j_n = \infty$. Introducing the limit in the above equation and using the asymptotic estimate for Legendre polynomials in [3] (2.117) we get

$$\lambda_\xi + \lim_{n \rightarrow \infty} \frac{\sum_{\zeta \in \mathcal{E} \setminus \{\xi\}} \lambda_\zeta P_{j_n}^d(\xi^T \zeta)}{P_{j_n}^d(1)} = 0.$$

This implies $\lambda_\xi = 0$ because the sum is finite and the latter part converges to zero.

Case 2 There is one $\zeta \in \mathcal{E}$ with $\xi^T \zeta = -1$.

Then ζ is the antipodal point of ξ and therefore in Cartesian coordinates $\zeta = -\xi$. Then the above equation becomes

$$\lambda_\xi P_j^d(1) + (-1)^j \lambda_{-\xi} P_j^d(1) + \sum_{\zeta \in \mathcal{E} \setminus \{\xi, -\xi\}} \lambda_\zeta P_j^d(\zeta^T \xi) = 0, \quad \forall j \in \mathcal{F}.$$

The third part vanishes if we introduce the limit as in the previous case but for odd and even series of j_n separately. The remainder yields for even j and odd j , respectively,

$$\lambda_\xi + \lambda_{-\xi} = 0 = \lambda_\xi - \lambda_{-\xi}$$

which implies $\lambda_\xi = 0 = \lambda_{-\xi}$. □

5 The Special Case of Kernels on the Circle

The case $d = 2$ is of special interest for us since the results of Theorem 4 do not apply to this case and since according to Lemma 6 (1) all axially symmetric kernels

on the circle have convolutional form. For $d = 2$ we note that a basis of the spherical harmonics is

$$Y_j(\xi) = \frac{1}{\sqrt{2\pi}} e^{ij\theta}, \quad j \in \mathbb{Z},$$

where θ is associated with the point on the circle $\xi = (\cos(\theta), \sin(\theta))^T \in \mathbb{S}^1$. The Legendre polynomials take the form of Chebyshev polynomials and the addition formula reads

$$Y_j(\xi)\bar{Y}_j(\zeta) + Y_{-j}(\xi)\bar{Y}_{-j}(\zeta) = \frac{2}{\pi} \cos(j(\theta - \nu)),$$

where θ is corresponding to ξ as above and $\zeta = (\cos(\nu), \sin(\nu))^T$. Using the circular harmonics every continuous kernel on $\mathbb{S}^1 \times \mathbb{S}^1$ has an expansion of the form

$$K(\xi, \zeta) = \sum_{j, j' \in \mathbb{Z}} a_{j, j'} e^{ij\theta} e^{-ij'\nu}.$$

For a Hermitian convolutional kernel only the coefficients corresponding to the same order of trigonometric polynomial are going to be non-zero. This yields

$$K(\xi, \zeta) = \sum_{j \in \mathbb{Z}_+} \left(d_{j, j} e^{ij(\theta - \nu)} + d_{-j, -j} e^{-ij(\theta - \nu)} + d_{-j, j} e^{-ij(\theta + \nu)} + \overline{d_{-j, j}} e^{ij(\theta + \nu)} \right) + d_{0, 0},$$

where we can define the matrices of the last section as $D_j = \begin{pmatrix} d_{j, j} & d_{j, -j} \\ \overline{d_{j, -j}} & d_{-j, -j} \end{pmatrix}$.

Theorem 5 *Let K be a continuous positive definite kernel of the form (26), $d = 2$, and \mathcal{F} be the corresponding index set for which the D_j are positive definite matrices. Then it is sufficient for K to be strictly positive definite that the set $\{n \in \mathbb{Z} \mid |n| \in \mathcal{F}\}$ intersects every full arithmetic progression in \mathbb{Z}_+ .*

Proof For this special case Lemma 13 (2) reads

$$\sum_{\xi \in \mathcal{E}} \lambda_\xi \cos\left(j \arccos(\xi^T \zeta)\right) = 0, \quad \forall j \in \mathcal{F}, \quad \forall \xi \in \mathbb{S}^1,$$

implies $\lambda_\xi = 0$ for all $\xi \in \mathcal{E}$. This is the case if all functions of the form $\sum_{j \in \mathcal{F}} a_j \cos(j \arccos(\xi^T \zeta))$ with $a_j > 0$ are positive definite and thereby we can deduce our result directly from Corollary 2.3 and Theorem 2.15 of [20]. \square

Theorem 6 *Let K be a continuous positive definite kernel of the form (26), $d = 2$ and \mathcal{J} the corresponding index set for which the D_j are non-zero. Then it is necessary for K to be strictly positive definite that \mathcal{J} intersects every full arithmetic progression in \mathbb{Z}_+ .*

Proof The proof again uses contradiction and the construction of sets which show that Lemma 13 (2) does not hold if \mathcal{J} does not intersect every full arithmetic progression. As in the previous cases this construction is the same which was used in the proof for isotropic kernels and we therefore refer to the proof of [4] Theorem 5.2, where details of the construction are given. \square

We briefly mention implications for kernel is axially symmetric kernels on \mathbb{S}^1 . According to Theorem 1, a kernel is axially symmetric if

$$a_{j,j'} = \delta_{j,j'} c_j.$$

Thereby a Hermitian axially symmetric kernel takes the form

$$K(\xi, \zeta) = \sum_{j \in \mathbb{Z}_+} \left(c_j e^{ij(\theta-\nu)} + c_{-j} e^{-ij(\theta-\nu)} \right) + c_0.$$

Then Theorems 5 and 6 directly apply to the axially symmetric kernels, where \mathcal{F} is the set of $j \in \mathbb{Z}$ for which both $c_j, c_{-j} > 0$ and \mathcal{J} is the set of indices j for which c_j or c_{-j} are non-zero.

6 Discussion

The discussion in Section 2 allows to construct kernels with different geometric properties. Even though these kernels could only be constructed approximately as truncated series we believe that they can nevertheless be used in applications as discussed in [2] for axially symmetric kernels. We also believe that taking into account a wider range of geometric properties of the kernel will allow the improvement of approximation results for many areas of application. Unfortunately any truncation would remove strict positive definiteness. This problem can be addressed in applications for example by choosing the truncation index high enough so that the remaining error is close to machine precision.

The more specific results in Section 3 show that stating necessary and sufficient conditions for axially symmetric strictly positive definite kernels is possible in a similar way to the results known for radial kernels and that in fact one can utilize the results known for isotropic kernels to prove the more general case, as done in Section 4.

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