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A NECESSARY AND SUFFICIENT CONDITION FOR STRICTLY POSITIVE DEFINITE FUNCTIONS ON SPHERES

DEBAO CHEN, VALDIR A. MENEGATTO, AND XINGPING SUN

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Abstract. We give a necessary and sufficient condition for the strict positive-definiteness of real and continuous functions on spheres of dimension greater than one.

1. Introduction

Let S^m $(m \geq 1)$ denote the unit sphere in the Euclidean space $\mathbb{R}^{m+1}$. Let x and y be two points on S^m, the usual geodesic distance between the two points is given by

$$d_m(x, y) = \operatorname{Arccos}(xy).$$

Here xy denotes the usual inner product of x and y. A continuous function $f : [0, \pi] \to R$ is said to be positive definite on S^m if, for any $N \in \mathbb{N}$ and any set of N points $x_1, \ldots, x_N$ in S^m, the $N \times N$ matrix A with ij entry $A_{ij} = (d_m(x_i, x_j))$ is nonnegative definite, i.e.,

$$c^T Ac = \sum_{i=1}^{N} \sum_{j=1}^{N} c_i c_j f(d_m(x_i, x_j)) \geq 0, \quad c = (c_1, \ldots, c_N) \in \mathbb{R}^N. \tag{1.1}$$

Schoenberg [S] characterized all the positive definite functions on S^m as those of the form

$$f(t) = \sum_{k=0}^{\infty} a_k P_k^{(\lambda)}(\cos t) \tag{1.2}$$

in which $\lambda = (m-1)/2$, $a_k \geq 0$, and $\sum a_k P_k^{(\lambda)}(1) < \infty$. Here $P_k^{(\lambda)}$ denotes the standard Gegenbauer polynomials (also called ultraspherical polynomials); see [Sz, p. 81].

Recently, there has been renewed interest in Schoenberg's result. With the motivation to employ positive definite functions in scattered data interpolation on spheres, Cheney introduced the notion of "strictly positive definite functions on S^m" in a lecture note. A positive definite function on S^m is said to be "strictly positive definite on S^m" if, for all $N \in \mathbb{N}$ and all sets of N **distinct** points $x_1, \ldots, x_N$,

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the matrices A in the above definition are positive definite, i.e., the quadratic forms in inequality (1.1) are positive for every nonzero vector $c \in \mathbb{R}^N$.

It is readily seen that the strict-positive-definiteness of a function f given in (1.2) depends only on the set

$$K_{m,f} := \{k \in \mathbb{Z}_+ : a_k > 0\},$$

but not on the actual values of the coefficients a_k. This fact motivates us to give the following definition.

Definition 1. A subset K of $\mathbb{Z}_+$ is said to induce strict-positive-definiteness (abbreviated as S.P.D.) on S^m if the function

$$t \mapsto \sum_{k \in K} P_k^{(\lambda)}(\cos t)$$

is strictly positive definite on S^m. Here and in what follows, we assume that a certain summation method has been applied here so that the series converges uniformly.

Xu and Cheney [XC] proved that the set $\mathbb{Z}_+$ induces S.P.D. on S^m. Schreiner [Sc] improved Xu and Cheney's result by showing that, for any fixed $N \in \mathbb{N}$, the set $\mathbb{Z}_+ \setminus \{0, 1, \ldots, N\}$ induces S.P.D. on S^m. Ron and Sun [RS1] linked this problem to multivariate polynomial interpolation, and proved several results, a corollary of which asserts that a subset K of $\mathbb{Z}_+$ induces S.P.D. on S^m if K contains arbitrarily long consecutive long strings of odd integers as well as arbitrarily long strings of consecutive even integers. In a series of publications by Menegatto [M1]-[M3], several necessary or sufficient conditions have been discussed.

In the present study, we give an if-and-only-if condition for a subset K of $\mathbb{Z}_+$ to induce S.P.D. on S^m for $m \geq 2$. Our theorem simply states that a subset K of $\mathbb{Z}_+$ induces S.P.D. on S^m for $m \geq 2$ if and only if K contains infinitely many odd integers as well as infinitely many even ones. We point out that the necessity of this condition had earlier been demonstrated by Menegatto [M1], and therefore we focus on the sufficiency part of the theorem in the present paper. It is not unexpected that this sufficient condition does not hold true for strictly positive definite functions on S^1, the unit circle in $\mathbb{R}^2$. The failure of our proof applying to the case $m = 1$ will become self-evident with the unfolding of the argument. We will make a brief discussion about the intriguing case $m = 1$ at the end of this paper.

The layout of this paper is as follows. In Section 2, we establish several equivalent conditions for strictly positive definite functions on S^m. In Section 3, we prove our major result.

2. Equivalent conditions

Let $k \in \mathbb{Z}_+$, and let $\mathcal{H}_k^0$ denote the space of all the homogeneous harmonic polynomials of degree k. Also, for any $K \subset \mathbb{Z}_+$, we set

$$\mathcal{H}_K := \sum_{k \in K} \mathcal{H}_k^0.$$

Recall that the restriction of a homogeneous harmonic polynomial in $\mathcal{H}_k^0$ to S^m is called a *spherical harmonic* of degree k. The Gegenbauer polynomials are connected

to spherical harmonics by the so-called "Summation Formula" (see Stein and Weiss [SW, Chap. 4]):

Let $\{Y_1^{(k)}, \dots, Y_{h_k}^{(k)}\}$ be an orthonormal basis for $\mathcal{H}_k^0$, h_k being the dimension of this space. Then there is a positive constant $c_{k,\lambda}$ such that, for all $x, y \in S^m$,

$$P_k^{(\lambda)}(xy) = c_{k,\lambda} \sum_{j=1}^{h_k} Y_j^{(k)}(x) Y_j^{(k)}(y). \tag{2.1}$$

A *polar form* of this formula plays a key role in the proof of the major result in the present paper. For $m = 1$, the polar version of this formula is simply the addition formula for the cosine function in elementary trigonometry. For $m \geq 2$, we can choose any point $p \in S^m$ as the pole, introduce an angular variable θ, and represent a point $x \in S^m$ in the following form:

$$x = (\cos\theta, \sin\theta\, x'), \qquad x' \in S^{m-1}, \quad \cos\theta = px.$$

Here x' is often interpreted as the "curvilinear projection" of x onto the "equator" of S^m, which is S^{m-1}. Writing $y \in S^m$ in the polar form

$$y = (\cos\phi, \sin\phi\, y'), \qquad y' \in S^{m-1}, \quad \cos\phi = py,$$

we have the following formula (see [A, p. 30]):

$$P_k^{(\lambda)}(xy) = \sum_{l=0}^{k} b(k,\lambda,l) Q_k^{(l)}(\theta) Q_k^{(l)}(\phi) P_l^{(\lambda-1/2)}(x'y'), \tag{2.2}$$

in which we have introduced the functions

$$Q_k^{(l)}(\theta) := (\sin\theta)^l P_{k-l}^{(\lambda+l)}(\cos\theta), \quad 0 \leq l \leq k.$$

In (2.2), all the numbers $b(k,\lambda,l)$ are positive. The exact values of these numbers are known; see [A, p. 30] for details. However, in this study, we only use the fact that these numbers are positive. Equation (2.2) is called the "addition formula for Gegenbauer polynomials". Xu and Cheney [XC] first applied this formula to study strictly positive definite functions on S^m.

That the two formulas (2.1) and (2.2) are equivalent can be verified by some inspired calculations. However, that is not our concern in the present study. Therefore, instead of elaborating on the equivalence of the two formulas, we choose to use both freely in this paper.

Theorem 2. *Let $K \subset \mathbb{Z}_+$, and assume $m \geq 2$. Then the following statements are equivalent:*

1. *K induces S.P.D. on S^m.*
2. *There is no nontrivial linear functional $\psi \in C(S^m)^*$ that has finite support and annihilates $\mathcal{H}_K$.*
3. *For any $N \in \mathbb{N}$ and any set of N distinct points $x_1, \dots, x_N$, the N functions*
$$x \mapsto \sum_{k \in K} P_k^{(\lambda)}(xx_j), \qquad j = 1, \dots, N,$$
are linearly independent.
4. *For any $N \in \mathbb{N}$ and any set of N distinct points $x_1, \dots, x_N$ represented in polar form*
$$x_i = (\cos\theta_i, \sin\theta_i\, x_i'),$$

if there are N real numbers c_j $(j = 1, \dots, N)$ such that

$$\sum_{j=1}^{n} c_j Q_k^{(l)}(\theta_j) P_l^{(\lambda-1/2)}(x'x'_j) = 0, \quad k \in K, \quad 0 \le l \le k,$$

then all the c_j $(j = 1, \dots, N)$ must be zero.

Proof. Using the summation formula for spherical harmonics, we can write

$$\begin{aligned}\sum_{i=1}^{N}\sum_{j=1}^{N} c_i c_j \sum_{k\in K} P_k^{(\lambda)}(x_i x_j) &= \sum_{k\in K} c_{\lambda,k} \sum_{l=1}^{h_k}\sum_{i=1}^{N}\sum_{j=1}^{N} c_i c_j Y_l^{(k)}(x_i) Y_l^{(k)}(x_j) \\ &= \sum_{k\in K} c_{\lambda,k} \sum_{l=1}^{h_k}\Big(\sum_{j=1}^{N} c_j Y_l^{(k)}(x_j)\Big)^2.\end{aligned}$$

Therefore,

$$\sum_{i=1}^{N}\sum_{j=1}^{N} c_i c_j \sum_{k\in K} P_k^{(\lambda)}(x_i x_j) = 0 \tag{2.3}$$

if and only if

$$\sum_{j=1}^{N} c_j Y_l^{(k)}(x_j) = 0, \quad k \in K, \quad l = 1, \dots, h_k.$$

Accordingly, if K does not induce S.P.D. on S^m, then there is a nonzero vector $c = (c_1, \dots, c_N) \in \mathbb{R}^N$ such that (2.3) holds true. Let $\psi \in C(S^m)^*$ be defined by

$$\psi(f) = \sum_{j=1}^{N} c_j f(x_j), \quad f \in C(S^m).$$

Then, ψ is supported on a nonempty subset of $\{x_1, \dots, x_N\}$, and it annihilates $\mathcal{H}_K$. The above argument can be reversed to finish the proof that conditions 1 and 2 are equivalent. To see the equivalence between conditions 2 and 3, we use the summation formula for spherical harmonics again, and write

$$\sum_{j=1}^{N} c_j \sum_{k\in K} P_k^{(\lambda)}(x x_j) = \sum_{k\in K} c_{\lambda,k} \sum_{l=1}^{h_k}\Big(\sum_{j=1}^{N} c_j Y_l^{(k)}(x_j)\Big) Y_l^{(k)}(x).$$

Now suppose that the N functions given in Theorem 2 (condition 3) are linearly dependent. Then there is a nonzero vector $c = (c_1, \dots, c_N) \in \mathbb{R}^N$ such that

$$0 = \sum_{j=1}^{N} c_j \sum_{k\in K} P_k^{(\lambda)}(x x_j) = \sum_{k\in K} c_{\lambda,k} \sum_{l=1}^{h_k}\Big(\sum_{j=1}^{N} c_j Y_l^{(k)}(x_j)\Big) Y_l^{(k)}(x). \tag{2.4}$$

It is well-known that any set of finitely many distinctive spherical harmonics are linearly independent on S^m. Therefore, we must have

$$\sum_{j=1}^{N} c_j Y_l^{(k)}(x_j) = 0, \quad k \in K, \quad l = 1, \dots, h_k.$$

This violates condition 2. The other implication is obvious from (2.4).

Finally, we use the addition formula for Gegenbauer polynomials to show the equivalence between conditions 3 and 4. We write

(2.5)

$$\sum_{j=1}^{N} c_j \sum_{k\in K} P_k^{(\lambda)}(xx_j) = \sum_{j=1}^{N} c_j \sum_{k\in K}\sum_{l=0}^{k} b(k,\lambda,l) Q_k^{(l)}(\theta_j) Q_k^{(l)}(\theta) P_l^{(\lambda-1/2)}(x'x_j')$$
$$= \sum_{k\in K}\sum_{l=0}^{k} b(k,\lambda,l)\Big[\sum_{j=1}^{N} c_j Q_k^{(l)}(\theta_j) P_l^{(\lambda-1/2)}(x'x_j')\Big] Q_k^{(l)}(\theta).$$

Thus, if there is a nonzero vector $c = (c_1, \dots, c_N)$ such that

$$\sum_{j=1}^{N} c_j Q_k^{(l)}(\theta_j) P_l^{(\lambda-1/2)}(x'x_j') = 0, \quad k \in K, \quad l = 0, 1, \dots, k,$$

then the N functions

$$x \mapsto \sum_{k\in K} P_k^{(\lambda)}(xx_j), \quad j = 1, \dots, N,$$

are linearly dependent. On the other hand, if there is a nonzero vector $c = (c_1, \dots, c_N)$ such that

$$\sum_{j=1}^{N} c_j \sum_{k\in K} P_k^{(\lambda)}(xx_j) = 0,$$

then (2.4) shows that, for each $k \in K$,

$$\sum_{j=1}^{N} c_j P_k^{(\lambda)}(xx_j) = 0.$$

Since for each $k \in K$, the $k+1$ functions $Q_k^{(l)}, \quad l = 0, 1, \dots, k$, are linearly independent, we see from (2.5) that

$$\sum_{j=1}^{N} c_j Q_k^{(l)}(\theta_j) P_l^{(\lambda-1/2)}(x'x_j') = 0, \quad k \in K, \quad l = 0, 1, \dots, k.$$

□

3. Main result and proof

Let x_i $(i = 1, \dots, N)$ be N distinct points in S^m $(m \geq 2)$. Suppose that a pole p has been chosen so that the points have the representations

$$x_i = (\cos\theta_i, \sin\theta_i\, x_i'), \qquad x_i' \in S^{m-1}, \quad \cos\theta_i = px_i.$$

Part 4 of Theorem 2 allows us to work with the x_i's belonging to S^{m-1}, a sphere of one lower dimension, which is the crux of the proof. However, the dimension reduction also brings an inconvenience: we now have to deal with those double-indexed functions $Q_k^{(l)}$, $k \in K$, $l = 0, 1, \dots, k$. While there is a seemingly abundant supply of functions at our disposal, it is indeed a situation in which we feel that more is less. We choose to use only those functions $Q_k^{(k)}$, $k \in K$, and the assumption that there are both sufficiently large odd k and even k in K. To this end, we need a careful selection of the pole for the curvilinear projection, paying particular attention to the antipodal pairs that may appear in x_i $(i = 1, \dots, N)$.

If for some $1 \le i, j \le N$, x_i and x_j are antipodal, i.e. $x_i = -x_j$, then for any chosen pole p, we have $px_i = -px_j$, implying that $\sin\theta_i = \sin\theta_j$. On the other hand, if there is no antipodal pair among these points, then we can select a pole p such that the N numbers $\sin\theta_i$ are all nonzero and distinctive. In fact, if $\sin\theta_i = \sin\theta_j$ for a pair of i, j with $i \ne j$, then we have $\cos\theta_i = \pm\cos\theta_j$, i.e. $p(x_i \pm x_j) = 0$. Since $x_i \pm x_j \ne 0$ (the points are distinct and there is no antipodal pair among them), those p that satisfy one of the equations form a hyper "great circle" of S^m that is a copy of S^{m-1}. Since there are only finitely many of those great circles, and their union is not all of S^m, we can then find a $p \in S^m$ that is neither in the union of these great circles nor in the set $\{x_1, \dots, x_N\}$. Under the polar system based on the pole p, the N numbers $\sin\theta_i$ are all nonzero and distinctive.

Theorem 3. *Let $K \subset \mathbb{Z}_+$. In order that K induce S.P.D. on S^m $(m \ge 2)$ it is necessary and sufficient that K contain infinitely many odd integers as well as infinitely many even integers.*

Proof. The necessity of the theorem was demonstrated by Menegatto [M1]. To prove the sufficiency, let N be an arbitrary natural number, and let $x_1, \dots, x_N$ be N distinct points in S^m. Using the procedure described in the beginning of this section, we can choose a pole p and establish a polar coordinate system so that, under this system, the N numbers $\sin\theta_i$ $(i = 1, \dots, N)$ form a set having the following properties:

(i) $\sin\theta_i > 0, \quad i = 1, \dots, N.$
(ii) $\sin\theta_i = \sin\theta_j$ $(i \ne j)$, if and only if $x_i = -x_j$.

Here

$$x_i = (\cos\theta_i, \sin\theta_i x_i'), \qquad x_i' \in S^{m-1}, \quad \cos\theta_i = px_i.$$

To show that K induces S.P.D. of order N on S^m, suppose that there are N real numbers c_j $(j = 1, \dots, N)$ such that

$$\sum_{j=1}^{N} c_j Q_k^{(l)}(\theta_j) P_l^{(\lambda-1/2)}(x'x_j'), \quad k \in K, \quad l = 0, 1, \dots, k.$$

Letting $l = k$, we have

$$\sum_{j=1}^{N} c_j (\sin\theta_j)^k P_k^{(\lambda-1/2)}(x'x_j') = 0, \qquad k \in K. \tag{3.1}$$

We will show that all the c_j $(j = 1, \dots, N)$ are zero under the assumption that K contains infinitely many odd integers as well as infinitely many even integers. We then use Theorem 2 to reach the conclusion of Theorem 3. We will do induction on N, the number of distinct points in question. The result is obviously true for the cases that $N = 1$ and $N = 2$ with the two points x_1, x_2 being antipodal, i.e. $x_1 = -x_2$. Suppose that the theorem is proved true for each case in which we have less than N distinctive points. Here $N \ge 3$ if there is an antipodal pair, or $N \ge 2$ otherwise. We will prove that it is also true when we have N distinctive points. Let $1 \le j_0 \le N$ be such that $\sin\theta_{j_0} \ge \sin\theta_j$. At this point, it is necessary to break the rest of the proof into two cases:

(a) The set $\{x_1, \dots, x_N\} \setminus \{x_{j_0}\}$ does not contain the antipodal point of x_{j_0}.
(b) The set $\{x_1, \dots, x_N\} \setminus \{x_{j_0}\}$ contains the antipodal point of x_{j_0}.

In case (a), we have $\sin\theta_{j_0} > \sin\theta_j,\ j \neq j_0$. Dividing both sides of (3.1) by $\sin\theta_{j_0}$, and setting $x' = x'_{j_0}$, we get

$$\sum_{j\neq j_0} c_j \Big(\frac{\sin\theta_j}{\sin\theta_{j_0}}\Big)^k P_k^{(\lambda-1/2)}(x'_{j_0}x'_j) + c_{j_0}P_k^{(\lambda-1/2)}(1) = 0, \qquad k \in K. \tag{3.2}$$

Since K contains infinitely many nonnegative integers, we can let $k \to \infty$ in (3.2). Note that there exists a δ $(0 < \delta < 1)$, such that

$$\Big(\frac{\sin\theta_j}{\sin\theta_{j_0}}\Big)^k |P_k^{(\lambda-1/2)}(x'_{j_0}x'_j)| \leq \delta^k \cdot P_k^{(\lambda-1/2)}(1) = \delta^k \frac{\Gamma(k+\lambda+1)}{\Gamma(k+1)\Gamma(\lambda+1)}.$$

The right-hand side of the above inequality approaches to zero when $k \to \infty$. Therefore, from (3.2), we have

$$c_{j_0}P_k^{(\lambda-1/2)}(1) \to 0.$$

This implies that $c_{j_0} = 0$. Hence (3.1) is reduced to

$$\sum_{j\neq j_0} c_j(\sin\theta_j)^k P_k^{(\lambda-1/2)}(x'x'_j) = 0, \qquad k \in K.$$

Note that there are only $(N-1)$ terms in the left-hand side of the above equation, and the $(N-1)$ numbers $\{\sin_j\ j \neq j_0\}$ still have properties (i) and (ii). We can use induction hypothesis to draw the conclusion that all c_j $(j = 1, \ldots, N)$ are zero.

In case (b), let us assume that x_{j_1} is the antipodal point of x_{j_0}, i.e. $x_{j_1} = -x_{j_0}$, where $0 \leq j_1 \leq N$, and of course, $j_0 \neq j_1$. We have, under this circumstance, that $\sin\theta_{j_0} = \sin\theta_{j_1}$, and $\sin\theta_{j_0} > \sin\theta_j,\ j \neq j_0, j_1$. Again, dividing both sides of (3.1) by $\sin\theta_{j_0}$, and setting $x' = x'_{j_0}$, we get

$$\begin{aligned}\sum_{j\neq j_0,j_1} c_j \Big(\frac{\sin\theta_j}{\sin\theta_{j_0}}\Big)^k P_k^{(\lambda-1/2)}(x'_{j_0}x'_j)& \\ + c_{j_0}P_k^{(\lambda-1/2)}(1) + c_{j_1}P_k^{(\lambda-1/2)}(-1) = 0, \qquad k \in K.&\end{aligned} \tag{3.3}$$

Note that the Gegebauer polynomials $P_k^{(\lambda-1/2)}$ are odd functions when k is odd and even functions when k is even. Separating the odd ks from the even ones, we write down the following two equations:

$$\begin{aligned}\sum_{j\neq j_0,j_1} c_j \Big(\frac{\sin\theta_j}{\sin\theta_{j_0}}\Big)^k P_k^{(\lambda-1/2)}(x'_{j_0}x'_j)& \\ + [c_{j_0} - c_{j_1}]P_k^{(\lambda-1/2)}(1) = 0, \qquad k \in K, \quad k \text{ is odd},&\end{aligned} \tag{3.4}$$

$$\begin{aligned}\sum_{j\neq j_0,j_1} c_j \Big(\frac{\sin\theta_j}{\sin\theta_{j_0}}\Big)^k P_k^{(\lambda-1/2)}(x'_{j_0}x'_j)& \\ + [c_{j_0} + c_{j_1}]P_k^{(\lambda-1/2)}(1) = 0, \qquad k \in K, \quad k \text{ is even}.&\end{aligned} \tag{3.5}$$

Since K contains infinitely many odd integers as well as infinitely many even integers, we can let $k \to \infty$ in both (3.4) and (3.5). The same argument used in proving case (a) shows that $c_{j_0} \pm c_{j_1} = 0$, implying $c_{j_0} = c_{j_1} = 0$. Also the induction hypothesis takes care of the rest of the issue. $\square$

At the end of this paper, we make a brief discussion about the case $m = 1$. Obviously, the dimension-reduction technique stops working, and therefore, a new approach is needed to characterize all the strictly positive definite functions on the unit circle. As we already mentioned in the Introduction, the condition of Theorem 3 is no longer sufficient (while it is still necessary). In fact, Ron and Sun [RS2] showed that the set $\{4k, 4k+1 : k \in \mathbb{Z}_+\}$ does not induce S.P.D. on S^1. After a rather lengthy period of research, we come to admit (with a high degree of reluctance) that the S.P.D. functions on S^1 are still defying an elegant characterization.

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Department of Computer Sciences, Oklahoma State University-Tulsa, Tulsa, Oklahoma 74106

E-mail address: cdebao@cs.okstate.edu

ICMC-Universidade de Sao Paulo, Caixa Postal 668, 13560-970 Sao Carlos SP, Brasil

E-mail address: menegatt@icmc.usp.br

Department of Mathematics, Southwest Missouri State University, Springfield, Missouri 65804

E-mail address: xis280f@smsu.edu