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Conditionally positive definite kernels on Euclidean domains ☆

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Abstract

This paper characterizes several classes of conditionally positive definite kernels on a domain Ω of either $\mathbb{R}^l$ or $\mathbb{C}^l$. Among the classes is that composed of strictly conditionally positive definite kernels. These kernels are known to be useful in the solution of variational interpolation problems on Ω. Our study covers the case in which Ω is the sphere S^{l-1} of $\mathbb{R}^l$ or a similar manifold. Among other things, our results imply that the characterization of (strict) conditional positive definiteness on Ω can be obtained from a characterization of (strict) positive definiteness on Ω. The bi-zonal strictly conditionally positive definite kernels on S^{l-1}, $l \geqslant 3$, are described.

Keywords: Conditionally positive definite kernels; Positive definite kernels; Domains; Spheres; Bi-zonal kernels

1. Introduction

Positive definite and related kernels are encountered in many problems involving the numerical treatment of functions of several variables. Usually, the function one has to deal with has the form

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$$s(x)=\sum_{j=1}^{n} c_j f\big(d(x,x_j)\big), \quad c_j\in\mathbb{C}, \tag{1.1}$$

where the points x_j belong to a certain domain Ω of $\mathbb{R}^l$ or $\mathbb{C}^l$, d is some sort of metric structure of the domain and $(x,y)\in\Omega^2\mapsto f(d(x,y))$ is an at least continuous, positive definite or related kernel [4]. A potentially important example we have in mind is that in which Ω is the unit sphere S^{l-1} of $\mathbb{R}^l$ and d is either the geodesic distance in S^{l-1} or the inner product of $\mathbb{R}^l$.

Conditionally positive definite kernels come into play when low-degree polynomials are added to s. To understand that, one needs to recall the most common notion of conditional positive definiteness. It does not involve either the structure of Ω or the space where it is sitting but it depends on a subspace $\mathcal{P}$ of Π, the space of polynomials in l variables with complex coefficients in the case $\Omega\subset\mathbb{R}^l$ and the space of polynomials in the variables z and $\bar{z}$, $z\in\mathbb{C}^l$, otherwise. As it will become clear ahead, we will need in fact the space obtained from $\mathcal{P}$ by restricting its elements to Ω. We will not distinguish between these two versions of the same space.

A Hermitian kernel $f\colon \Omega\times\Omega\mapsto\mathbb{C}$ is *conditionally positive definite with respect to* $\mathcal{P}$ on Ω if for all $\{x_1,\ldots,x_n\}\subset\Omega$, and $\{c_1,\ldots,c_n\}\subset\mathbb{C}$ satisfying

$$\sum_{\mu=1}^{n} c_\mu p(x_\mu)=0, \quad p\in\mathcal{P}, \tag{1.2}$$

the associated quadratic form

$$\sum_{\mu,\nu=1}^{n} c_\mu\bar{c}_\nu f(x_\mu,x_\nu) \tag{1.3}$$

is nonnegative. If the quadratic form is positive when the x_j are distinct, the c_μ satisfy (1.2) and $\sum_{\mu=1}^{n}|c_\mu|>0$, then the kernel f is called *strictly conditionally positive definite with respect to* $\mathcal{P}$ on Ω. A (*strictly*) *positive definite* kernel on Ω is then a (strictly) conditionally positive definite kernel with respect to the trivial subspace $\{0\}$ on Ω.

If a kernel f is strictly conditionally positive definite with respect to a finite-dimensional subspace $\mathcal{P}$ of Π, then the interpolation problem

$$\sum_{\nu=1}^{n} c_\nu f(x_\mu,x_\nu)+q(x_\mu)=\lambda_\mu, \quad \mu=1,\ldots,n,\ q\in\mathcal{P}, \tag{1.4}$$

under the condition

$$\sum_{\nu=1}^{n} c_\nu p(x_\nu)=0, \quad p\in\mathcal{P}, \tag{1.5}$$

is always uniquely soluble as long as $p=0$ is the only element of $\mathcal{P}$ vanishing at the interpolation points. In applications, the most common setting where conditionally positive definite kernels appear is the real one while the space $\mathcal{P}$ is always finite dimensional. The usual choice for $\mathcal{P}$ is the space of polynomials of degree at most m, for some m.

Conditional positive definiteness with respect to $\mathcal{P}$ on Ω is then termed conditional positive definiteness of order m on Ω. We refer to [4,12] and references therein for general information on conditionally positive definite kernels on subsets of $\mathbb{R}^l$.

The purpose of this paper is to introduce and characterize two classes of conditionally positive definite kernels, including the strict cases. To better explain that, we first introduce the basic setting adopted in the whole paper.

Let Ω be a quite general subset of either $\mathbb{R}^l$ or $\mathbb{C}^l$ and $d\omega$ a positive measure on Ω not concentrated on a subset of Ω of measure zero. We will not list any additional hypothesis on either Ω or ω but our intention is to avoid singular cases. We will assume that the space $L^2(\Omega, d\omega)$ possesses an ordered countable basis $\{\varphi_k\}$, orthonormal with respect to the inner product $\langle\cdot,\cdot\rangle$ of $L^2(\Omega, d\omega)$, that is,

$$\int_\Omega \varphi_j(x)\overline{\varphi_k(x)}\, d\omega(x) = \delta_{jk}, \quad j,k = 0,1,\ldots. \tag{1.6}$$

For the cases we are specially interested, the basis $\{\varphi_k\}$ can be assumed to be in the space

$$\Pi|_\Omega := \{p|_\Omega\colon\ p \in \Pi\}. \tag{1.7}$$

Thus, in addition to the above, we will assume that every member of the family is a continuous function, even knowing that such assumption may be not needed in many places in the paper.

We will deal with kernels having an absolutely and uniformly convergent series representation in the form

$$f(x,y) = \sum_{k=0}^{\infty} a_k(f)\varphi_k(x)\overline{\varphi_k(y)}, \quad x,y \in \Omega. \tag{1.8}$$

The Fourier coefficients of f in (1.8) are given by

$$a_k(f) := \int_\Omega\int_\Omega f(x,y)\overline{\varphi_k(x)}\,\varphi_k(y)\, d\omega(x)\, d\omega(y). \tag{1.9}$$

One class of kernels is then $CPD_{\mathcal{P}}(\Omega)$, the set of kernels that are both, representable as in (1.8) and conditionally positive definite with respect to $\mathcal{P}$ on Ω. Its subclass $SCPD_{\mathcal{P}}(\Omega)$ is that comprising the elements of $CPD_{\mathcal{P}}(\Omega)$ which are strictly conditionally positive definite kernels with respect to $\mathcal{P}$ on Ω.

To proceed, we make use of the orthogonal complement of a subspace of Π. Precisely, given a subspace $\mathcal{P}$ of Π we write

$$\mathcal{P}^\perp := \big\{q \in L^2(\Omega, d\omega)\colon\ \langle q,p\rangle = 0,\ p \in \mathcal{P}\big\}. \tag{1.10}$$

A kernel f is *integrally conditionally positive definite with respect to* $\mathcal{P}$ on Ω if the following condition holds:

$$\int_\Omega\int_\Omega f(x,y)\overline{h(x)}\,h(y)\, d\omega(x)\, d\omega(y) \geqslant 0, \quad h \in C(\Omega)\cap\mathcal{P}^\perp, \tag{1.11}$$

where $C(\Omega)$ stands for the space of continuous functions on Ω. It is *strictly integrally conditionally positive definite with respect to* $\mathcal{P}$ on Ω if the inequality in (1.11) is strict when $h \in (C(\Omega) \cap \mathcal{P}^{\perp}) \setminus \{0\}$. These two classes of kernels will be denoted, respectively, by $ICPD_{\mathcal{P}}(\Omega)$ and $SICPD_{\mathcal{P}}(\Omega)$. In our context, it will become clear that these two concepts of integral conditional positive definiteness are easier to handle than the previous ones. As expected, in most cases $ICPD_{\mathcal{P}}(\Omega) \subset CPD_{\mathcal{P}}(\Omega)$ and $SICPD_{\mathcal{P}}(\Omega) \subset SCPD_{\mathcal{P}}(\Omega)$.

The paper is laid out as follows. In Section 2 we fully characterize the classes $CPD_{\mathcal{P}}(\Omega)$ and $ICPD_{\mathcal{P}}(\Omega)$. In the case Ω is a real sphere, this result generalizes a famous theorem of Schoenberg [15] concerning zonal positive definite functions on spheres. One of the inclusions mentioned in the previous paragraph is plainly justified. The rest of the section investigates conditions under which the reverse inclusion holds. Section 3 investigates the classes $SCPD_{\mathcal{P}}(\Omega)$ and $SICPD_{\mathcal{P}}(\Omega)$, including a characterization of the latter. It contains another major result of the paper which asserts that the class $SCPD_{\mathcal{P}}(\Omega)$ can be described as long as a description of $SCPD_{\{0\}}(\Omega)$ is available. In Section 4, we specialize the results in Sections 2 and 3 to the case in which $\Omega = S^{l-1}$. The classes $\mathcal{Z}_l \cap CPD_{\mathcal{P}}(S^{l-1})$ and $\mathcal{Z}_l \cap SCPD_{\mathcal{P}}(S^{l-1})$, where $\mathcal{Z}_l$ denotes the class of bi-zonal kernels on S^{l-1}, are identified for all values of l, but one, and for many choices of the space $\mathcal{P}$. In Section 5, we go one step further, extending the results in Section 4 to the case in which $\Omega = \Omega_{2l}$, the unit sphere in $\mathbb{C}^l$.

2. Conditional positive definiteness

In many interesting cases, including the case in which Ω is a sphere or a spherical surface, the orthonormal basis $\{\varphi_k\}$ can be taken polynomial. When this is not the case, we will require the basis to contain a basis of the polynomial space $\mathcal{P}$. The reason why this is an aspect that should not be ignored is the following

Lemma 2.1. *Let $\mathcal{P}$ be a subspace of Π. The following assertions hold*:

(i) *If $\varphi_k \in \mathcal{P}^{\perp}$ then $\varphi \notin \mathcal{P}$*;
(ii) *If $\{\varphi_k\}$ contains a basis for $\mathcal{P}$ and $\varphi_j \notin \mathcal{P}$ for some j then $\varphi_j \in \mathcal{P}^{\perp}$.*

A first relationship among the classes we have introduced so far is formalized below.

Theorem 2.2. *Let $\mathcal{P}$ be a subspace of Π. If $\{\varphi_k\}$ contains a basis for $\mathcal{P}$ then $ICPD_{\mathcal{P}}(\Omega) \subset CPD_{\mathcal{P}}(\Omega)$.*

Proof. If $f \in ICPD_{\mathcal{P}}(\Omega)$, then $a_k(f) \geqslant 0$ when $\varphi_k \in \mathcal{P}^{\perp}$. If, in addition, $\{\varphi_k\}$ contains a basis for $\mathcal{P}$ then Lemma 2.1 reveals that the previous conclusion corresponds to $a_k(f) \geqslant 0$, $\varphi_k \notin \mathcal{P}$. That $f \in CPD_{\mathcal{P}}(\Omega)$ now follows by calculating the quadratic form (1.3). □

Next, we present conditions under which the converse of Theorem 2.2 is true. The converse itself appears in Theorem 2.6, after we recall some basics about the concept of Lagrange-type bases and state two auxiliary results.

Let $\mathcal{P}$ be a finite-dimensional subspace of Π, m its dimension and $\{y_1, \dots, y_m\}$ a subset of Ω. A *Lagrange-type basis* for $\mathcal{P}$ with respect to $\{y_1, \dots, y_m\}$ is a basis $\{q_1, \dots, q_m\}$ of $\mathcal{P}$ such that $q_j(y_i) = \delta_{ij}$. The construction of a Lagrange-type basis usually begins with the choice of a basis $\{p_1, \dots, p_m\}$ for $\mathcal{P}$. Then one chooses a subset $\Gamma = \{y_1, \dots, y_m\}$ of Ω such that the linear functionals

$$p \in \mathcal{P} \mapsto p(y_j), \quad j = 1, \dots, m, \tag{2.1}$$

form a linearly independent set. This can be done by induction selecting Γ so that the matrix $P(y_1, \dots, y_m) := (p_i(y_j))$ and its principal minors have nonzero determinant. Such a set is called a *fundamental set* of $\mathcal{P}$. Finally, the set $\{q_1, \dots, q_m\}$ in which

$$q_i(x) := \frac{\det P(y_1, \dots, y_{i-1}, x, y_{i+1}, \dots, y_m)}{\det P(y_1, \dots, y_{i-1}, y_i, y_{i+1}, \dots, y_m)}, \quad i = 1, \dots, m, \tag{2.2}$$

is a Lagrange-type basis with respect to Γ.

Lemma 2.3 and Theorem 2.4 below provide a method to derive a kernel in $CPD_{\{0\}}(\Omega)$ from a kernel in $CPD_{\mathcal{P}}(\Omega)$. The ideas behind these two results are originally from the theory of positive definite functions on groups (see Chapter 3 in [2]) and have strong connections with reproducing kernel Hilbert spaces. Early papers of I.J. Schoenberg [13,14] also made use of similar relations between different types of kernels. Our proof of Theorem 2.4 is a simplified version of arguments explored in [12].

Lemma 2.3. *Let $\mathcal{P}$ be an m-dimensional subspace of Π, $\Gamma = \{y_1, \dots, y_m\}$ a subset of Ω and $\{q_1, \dots, q_m\}$ a basis for $\mathcal{P}$. If f is as in* (1.8) *and*

$$\begin{aligned} g(x, y) := f(x, y) - \sum_{i=1}^{m} q_i(x) f(y_i, y) - \sum_{j=1}^{m} \overline{q_j(y)} f(x, y_j) \\ + \sum_{i=1}^{m} \sum_{j=1}^{m} q_i(x) \overline{q_j(y)} f(y_i, y_j), \end{aligned} \tag{2.3}$$

then $a_k(g) = a_k(f)$, $\varphi_k \in \mathcal{P}^{\perp}$.

Proof. Direct computation with formula (1.9) with a help of the orthonormality of $\{\varphi_k\}$. $\square$

Theorem 2.4. *Let $\mathcal{P}$ and Γ be as in the previous lemma and $\{q_1, \dots, q_m\}$ a Lagrange-type basis for $\mathcal{P}$ with respect to Γ. Then the following assertions hold*:

(i) *If $f \in CPD_{\mathcal{P}}(\Omega)$ then the kernel g, as described in Lemma* 2.3*, is an element of $CPD_{\{0\}}(\Omega)$*;

(ii) *If $f \in SCPD_{\mathcal{P}}(\Omega)$ then $g \in SCPD_{\{0\}}(\Omega \setminus \Gamma)$.*

Proof. (i) Let $\{x_1, \dots, x_n\} \subset \Omega$ and $\{c_1, \dots, c_n\} \subset \mathbb{C}$. The quadratic form

$$Q := \sum_{\mu,\nu=1}^{n} c_\mu \bar{c}_\nu g(x_\mu, x_\nu) \tag{2.4}$$

can be decomposed in the form

$$\sum_{\mu,\nu=1}^{n} c_\mu \bar{c}_\nu f(x_\mu, x_\nu) - \sum_{i=1}^{m}\sum_{\nu=1}^{n} \bar{c}_\nu b_i f(y_i, x_\nu) - \sum_{j=1}^{m}\sum_{\mu=1}^{n} c_\mu \bar{b}_j f(x_\mu, y_j) + \sum_{i,j=1}^{m} b_i \bar{b}_j f(y_i, y_j), \tag{2.5}$$

in which

$$b_i = \sum_{j=1}^{n} c_j q_i(x_j), \quad i = 1, \dots, m. \tag{2.6}$$

Hence,

$$Q = \sum_{\mu,\nu=1}^{m+n} a_\mu \bar{a}_\nu f(w_\mu, w_\nu), \tag{2.7}$$

where

$$a_\mu = \begin{cases} c_\mu, & \mu = 1, \dots, n, \\ -b_{\mu-n}, & \mu = n+1, \dots, m+n, \end{cases} \tag{2.8}$$

and

$$w_\mu = \begin{cases} x_\mu, & \mu = 1, \dots, n, \\ y_{\mu-n}, & \mu = n+1, \dots, m+n. \end{cases} \tag{2.9}$$

It is now clear that the proof will be completed as long as we show that

$$\sum_{\mu=1}^{m+n} a_\mu q_k(w_\mu) = 0, \quad k = 1, \dots, m. \tag{2.10}$$

But, using (2.6) and the fact that $\{q_1, \dots, q_n\}$ is a Lagrange-type basis for $\mathcal{P}$ yield

$$\sum_{\mu=1}^{m+n} a_\mu q_k(w_\mu) = \sum_{\mu=1}^{n} c_\mu q_k(x_\mu) - \sum_{\mu=1}^{m} b_\mu q_k(y_\mu) = b_k - b_k = 0, \quad k = 1, \dots, m. \tag{2.11}$$

(ii) Assume that at least one c_μ is nonzero and that $\{x_1, \dots, x_n\} \subset \Omega \setminus \Gamma$. Then at least one a_μ is nonzero and the w_μ are pairwise distinct. Thus, if $f \in SCPD_{\mathcal{P}}(\Omega)$, the quadratic form in (2.7) is positive. □

Corollary 2.5. *Under the conditions in Theorem* 2.4*, the following assertions hold for a subspace $\mathcal{P}_1$ of $\mathcal{P}$:*

(i) *If $f \in CPD_{\mathcal{P}}(\Omega)$ then the kernel g, as defined in Lemma* 2.3*, is an element of $CPD_{\mathcal{P}_1}(\Omega)$;*
(ii) *If $f \in SCPD_{\mathcal{P}}(\Omega)$ then $g \in SCPD_{\mathcal{P}_1}(\Omega \setminus \Gamma)$.*

Proof. It suffices to use the previous theorem along with the inclusions $CPD_{\{0\}}(\Omega) \subset CPD_{\mathcal{P}_1}(\Omega)$ and $SCPD_{\{0\}}(\Omega \setminus \Gamma) \subset SCPD_{\mathcal{P}_1}(\Omega \setminus \Gamma)$. □

Theorem 2.6. *If $\mathcal{P}$ is a finite-dimensional subspace of Π then $CPD_{\mathcal{P}}(\Omega) \subset ICPD_{\mathcal{P}}(\Omega)$.*

Proof. Select a Lagrange-type basis $\{q_1, \ldots, q_m\}$ for $\mathcal{P}$ with respect to a subset $\Gamma = \{y_1, \ldots, y_m\}$ of Ω. Let $f \in CPD_{\mathcal{P}}(\Omega)$ and consider g as defined in Lemma 2.3. Since $g \in CPD_{\{0\}}(\Omega)$, the inequality

$$\sum_{\mu=1}^{n} |c_\mu|^2 f(x_\mu, x_\mu) + \sum_{\substack{\mu,\nu=1\\ \mu\neq\nu}}^{n} \bar{c}_\mu c_\nu f(x_\mu, x_\nu) - \sum_{i=1}^{m}\left(\sum_{\mu=1}^{n} \bar{c}_\mu q_i(x_\mu)\right)\sum_{\nu=1}^{n} c_\nu f(y_i, x_\nu)$$
$$- \sum_{j=1}^{m}\left(\sum_{\nu=1}^{n} c_\nu \overline{q_j(x_\nu)}\right)\sum_{\mu=1}^{n} \bar{c}_\mu f(x_\mu, y_j)$$
$$+ \sum_{i=1}^{m}\sum_{j=1}^{m} f(y_i, y_j)\left(\sum_{\mu=1}^{n} \bar{c}_\mu q_i(x_\mu)\right)\left(\sum_{\nu=1}^{n} c_\nu \overline{q_j(x_\nu)}\right) \geqslant 0$$

holds for $\{c_1, \ldots, c_n\} \subset \mathbb{C}$ and $\{x_1, \ldots, x_n\} \subset \Omega$. In particular,

$$\sum_{\mu=1}^{n} \left|h(x_\mu)\right|^2 f(x_\mu, x_\mu) + \sum_{\substack{\mu,\nu=1\\ \mu\neq\nu}}^{n} \overline{h(x_\mu)} h(x_\nu) f(x_\mu, x_\nu)$$
$$- \sum_{i=1}^{m}\left(\sum_{\mu=1}^{n} \overline{h(x_\mu)} q_i(x_\mu)\right)\sum_{\nu=1}^{n} h(x_\nu) f(y_i, x_\nu)$$
$$- \sum_{j=1}^{m}\left(\sum_{\nu=1}^{n} h(x_\nu)\overline{q_j(x_\nu)}\right)\sum_{\mu=1}^{n} \overline{h(x_\mu)}\, f(x_\mu, y_j)$$
$$+ \sum_{i=1}^{m}\sum_{j=1}^{m} f(y_i, y_j)\left(\sum_{\mu=1}^{n} \overline{h(x_\mu)} q_i(x_\mu)\right)\left(\sum_{\nu=1}^{n} h(x_\nu)\overline{p_j(x_\nu)}\right) \geqslant 0$$

holds for $h \in C(\Omega) \cap \mathcal{P}^\perp$ and $\{x_1, \ldots, x_n\} \subset \Omega$. Integration with respect to x_μ and x_ν yield

$$\omega(\Omega) \sum_{\mu=1}^{n} \int_\Omega \left|h(x_\mu)\right|^2 f(x_\mu, x_\mu)\, d\omega(x_\mu)$$
$$+ \sum_{\substack{\mu,\nu=1\\ \mu\neq\nu}}^{n} \int_\Omega \int_\Omega f(x_\mu, x_\nu)\overline{h(x_\mu)}\, h(x_\nu)\, d\omega(x_\mu)\, d\omega(x_\nu) \geqslant 0, \tag{2.12}$$

in which $\omega(\Omega)$ stands for the measure of Ω. Defining $M := \max\{f(x_\mu, x_\mu)\colon\ \mu = 1, \ldots, n\}$, the above inequality implies that

$$nM\omega(\Omega) \int_\Omega \left|h(x)\right|^2 d\omega(x) + n(n-1) \int_\Omega \int_\Omega f(x, y)\overline{h(x)} h(y)\, dw(x)\, d\omega(y) \geqslant 0. \tag{2.13}$$

Dividing by $n(n-1)$ and letting $n \to \infty$, we obtain

$$\int_\Omega \int_\Omega f(x, y)\overline{h(x)}h(y)\, d\omega(x)\, d\omega(y) \geqslant 0, \tag{2.14}$$

concluding the proof of the theorem. □

The following theorem is now evident.

Theorem 2.7. *Let $\mathcal{P}$ be a finite-dimensional subspace of Π. Assume $\{\varphi_k\}$ contains a basis for $\mathcal{P}$. Then the following assertions are equivalent*:

(i) $f \in CPD_{\mathcal{P}}(\Omega)$;
(ii) $f \in ICPD_{\mathcal{P}}(\Omega)$;
(iii) $a_k(f) \geqslant 0$, $\varphi_k \in \mathcal{P}^\perp$;
(iv) $a_k(f) \geqslant 0$, $\varphi_k \notin \mathcal{P}$.

Proof. Theorem 2.6 shows that (i) implies (ii). That (iii) follows from (ii) is obvious. Lemma 2.1(ii) justifies that (iii) implies (iv). The closing implication follows by direct computation. □

References [8,10] contain some interesting discussion on the connection between positive definite and integrally positive definite kernels.

3. Strict conditional positive definiteness

As it turns out, strict integral conditional positive definiteness is not difficult to describe. Before we do that, let us introduce the truncated series of a kernel f representable as in (1.8) with respect to a subspace $\mathcal{P}$ of Π. It is just

$$f_{\mathcal{P}}^{\perp}(x, y) := \sum_{k:\ \varphi_k \notin \mathcal{P}} a_k(f)\varphi_k(x)\overline{\varphi_k(y)}, \quad x, y \in \Omega. \tag{3.1}$$

The importance of this notion for conditional positive definiteness is illustrated by the following lemma whose proof will be omitted.

Lemma 3.1. *Let $\mathcal{P}$ be a subspace of Π and let $\mathcal{F}$ denote any of the classes $CPD_{\mathcal{P}}(\Omega)$, $SCPD_{\mathcal{P}}(\Omega)$, $ICPD_{\mathcal{P}}(\Omega)$ and $SICPD_{\mathcal{P}}(\Omega)$. Then $f_{\mathcal{P}}^{\perp} \in \mathcal{F}$ if and only if $f \in \mathcal{F}$.*

Theorem 3.2 below reveals that strict integral conditional positive definiteness is the best one can expect when dealing with strict conditional positive definiteness.

Theorem 3.2. *Let $\mathcal{P}$ be a subspace of Π and f a kernel as in* (1.8). *The following assertions are equivalent*:

(i) $f \in SICPD_{\mathcal{P}}(\Omega)$;
(ii) $a_k(f) > 0$ *whenever* $\varphi_k \in \mathcal{P}^\perp$.

Proof. One implication is obvious since we can replace h by φ_k in (1.11). Conversely, assume that $a_k(f) > 0$ when $\varphi_k \in \mathcal{P}^\perp$ and suppose that $f \notin ISCPD_{\mathcal{P}}(\Omega)$. Due to Lemma 3.1, we conclude that

$$\int_\Omega \int_\Omega f_{\mathcal{P}}^\perp(x,y)\overline{h(x)}\,h(y)\,d\omega(x)\,d\omega(y) = 0 \tag{3.2}$$

for some $h \in (C(\Omega) \cap \mathcal{P}^\perp) \setminus \{0\}$. Since $\{\varphi_k\}$ is an orthonormal basis for $L^2(\Omega, d\omega)$, there is $\varphi_{k_0} \notin \mathcal{P}$ such that $\langle \varphi_{k_0}, h\rangle \neq 0$. It follows that

$$0 = \int_\Omega \int_\Omega f_{\mathcal{P}}^\perp(x,y)\overline{h(x)}\,h(y)\,d\omega(x)\,d\omega(y) \geqslant \langle \varphi_{k_0}, h\rangle \overline{\langle \varphi_{k_0}, h\rangle} > 0, \tag{3.3}$$

a contradiction. □

Next, we turn to plain strict conditional positive definiteness with respect to $\mathcal{P}$. It is not hard to see that the strict conditional positive definiteness of a kernel $f \in CPD_{\mathcal{P}}(\Omega)$ depends upon the set

$$A_{\mathcal{P}}(f) := \{k\colon \varphi_k \notin \mathcal{P}\} \cap \big\{k\colon a_k(f) > 0\big\} \tag{3.4}$$

and not on the actual values of the coefficients $a_k(f)$. Thus, the following definition needs no additional explanation: let $\mathcal{L}$ be a family of subsets of $\mathbb{Z}_+$ and $\mathcal{F}$ a subset of $SCPD_{\mathcal{P}}(\Omega)$. We say that $\mathcal{L}$ *represents* $\mathcal{F}$ if the following two conditions hold:

(i) If $f \in \mathcal{F}$, there exists $K \in \mathcal{L}$ such that $A_{\mathcal{P}}(f) = K$;
(ii) If $K \in \mathcal{L}$, there exists $f \in \mathcal{F}$ such that $K = A_{\mathcal{P}}(f)$.

It is known that for some choices of Ω and $\mathcal{P}$ (see the case $\Omega = S^{l-1}$ in [4]), kernels in $SCPD_{\mathcal{P}}(\Omega)$ have the following invariance property: if $f \in SCPD_{\mathcal{P}}(\Omega)$ and $m \geqslant 0$ then any kernel $g \in CPD_{\mathcal{P}}(\Omega)$ such that

$$A_{\mathcal{P}}(g) = A_{\mathcal{P}}(f) + m := \big\{\alpha + m\colon \alpha \in A_{\mathcal{P}}(f)\big\} \tag{3.5}$$

belongs to $SCPD_{\mathcal{P}}(\Omega)$. This property is the motivation to our next definition. A family $\mathcal{L}$ of subsets of $\mathbb{Z}_+$ is *translation-invariant* if it possesses the following feature: if $K \in \mathcal{L}$ and A is finite then $K \setminus A \in \mathcal{L}$.

The following lemma complements Lemma 2.3 and Theorem 2.4.

Lemma 3.3. *Let $\mathcal{P}$, Γ, $\{q_1, \ldots, q_m\}$, f and g be as in Lemma* 2.3. *If*

$$h(x,y) := g(x,y) + \sum_{j=1}^{m} q_j(x)\overline{q_j(y)}, \quad x, y \in \Omega, \tag{3.6}$$

then $a_k(h) = a_k(g)$ when $\varphi_k \in \mathcal{P}^\perp$. If $\{q_1, \ldots, q_m\}$ is a Lagrange-type basis for $\mathcal{P}$ with respect to Γ and $f \in CPD_{\mathcal{P}}(\Omega)$ then $h \in CPD_{\{0\}}(\Omega)$. Further, if $f \in SCPD_{\mathcal{P}}(\Omega)$ then $h \in SCPD_{\{0\}}(\Omega)$.

Proof. The first assertion of the lemma is obvious. To prove the others, assume that $\{q_1, \dots, q_m\}$ is a Lagrange-type basis for $\mathcal{P}$ with respect to Γ and let $\{x_1, \dots, x_n\} \subset \Omega$ and $\{c_1, \dots, c_n\} \subset \mathbb{C}$. Then, the quadratic form $R := \sum_{\mu,\nu=1}^n c_\mu \bar{c}_\nu h(x_\mu, x_\nu)$ can be written as

$$R = \sum_{\mu,\nu=1}^n c_\mu \bar{c}_\nu g(x_\mu, x_\nu) + \sum_{j=1}^m \left| \sum_{\mu=1}^n c_\mu q_j(x_\mu) \right|^2. \tag{3.7}$$

If $f \in CPD_{\mathcal{P}}(\Omega)$, Theorem 2.4(i) implies that $g \in CPD_{\{0\}}(\Omega)$. Hence, $R \geqslant 0$, and consequently, $h \in CPD_{\{0\}}(\Omega)$. To finish the proof, assume the x_μ are distinct. The condition $R = 0$ yields the conclusions

$$\sum_{\mu=1}^n c_\mu q_j(x_\mu) = 0, \quad 1 \leqslant j \leqslant m, \tag{3.8}$$

and

$$\sum_{\mu,\nu=1}^n c_\mu \bar{c}_\nu g(x_\mu, x_\nu) = 0. \tag{3.9}$$

Looking at the definition of g, we obtain

$$\sum_{\mu,\nu=1}^n c_\mu \bar{c}_\nu f(x_\mu, x_\nu) = \sum_{\mu,\nu=1}^n c_\mu \bar{c}_\nu g(x_\mu, x_\nu) = 0. \tag{3.10}$$

Hence, if $f \in SCPD_{\mathcal{P}}(\Omega)$, Eq. (3.10) implies that $c_1 = \dots = c_n = 0$, therefore $h \in SCPD_{\{0\}}(\Omega)$. $\square$

Regarding the kernels involved in Lemma 2.3, Theorem 2.4 and Lemma 3.3, the following formulas hold when $\{\varphi_k\}$ contains a basis for $\mathcal{P}$:

$$a_k(g) = a_k(f) - \langle f(y_k, \cdot), \bar{p}_k \rangle - \langle f(\cdot, y_k), p_k \rangle + f(y_k, y_k), \quad \varphi_k \notin \mathcal{P}^\perp, \tag{3.11}$$

and $a_k(h) = a_k(g) + 1$, $\varphi_k \notin \mathcal{P}^\perp$. Even being interesting, these formulas will be of no use in this paper.

The major theorem in this paper is as follows.

Theorem 3.4. *Let $\mathcal{P}$ be an m-dimensional subspace of Π and $\mathcal{P}_1$ a subspace of $\mathcal{P}$. Assume $\{\varphi_k\}$ contains a basis for $\mathcal{P}$. If $\mathcal{L}$ is a translation-invariant family that represents $SCPD_{\mathcal{P}_1}(\Omega)$ then $\{K \in \mathcal{L}\colon\ K \cap \{k\colon\ \varphi_k \in \mathcal{P}\} = \emptyset\}$ represents $SCPD_{\mathcal{P}}(\Omega)$.*

Proof. Let $f \in SCPD_{\mathcal{P}}(\Omega)$. Choose a Lagrange-type basis $\{q_1, \dots, q_m\}$ for $\mathcal{P}$ with respect to a subset $\Gamma = \{y_1, \dots, y_m\}$ of Ω and consider the corresponding kernel h given in (3.6). Due to Lemma 3.3 and Corollary 2.5, $h \in SCPD_{\mathcal{P}_1}(\Omega)$. By Lemma 3.1, $h^\perp_{\mathcal{P}_1} \in SCPD_{\mathcal{P}_1}(\Omega)$ while the translation-invariance of $\mathcal{L}$ guarantees that $h^\perp_{\mathcal{P}} \in SCPD_{\mathcal{P}_1}(\Omega)$. Since $\mathcal{L}$ represents the family $SCPD_{\mathcal{P}_1}(\Omega)$, there exists $A \in \mathcal{L}$ such that $A_{\mathcal{P}_1}(h^\perp_{\mathcal{P}}) = A$. Lemma 3.3 implies that

$$a_k(h) = a_k(f), \quad \varphi_k \in \mathcal{P}^\perp. \tag{3.12}$$

Since $\{\varphi_k\}$ contains a basis for $\mathcal{P}$, it follows that

$$a_k(h) = a_k(f), \quad \varphi_k \notin \mathcal{P}. \tag{3.13}$$

Hence,

$$\begin{aligned} A_{\mathcal{P}_1}\big(h_{\mathcal{P}}^{\perp}\big) &= \{k\colon \varphi_k \notin \mathcal{P}_1\} \cap \big\{k\colon a_k\big(h_{\mathcal{P}}^{\perp}\big) > 0\big\} \\ &= \{k\colon \varphi_k \notin \mathcal{P}\} \cap \big\{k\colon a_k\big(h_{\mathcal{P}}^{\perp}\big) > 0\big\} \\ &= \{k\colon \varphi_k \notin \mathcal{P}\} \cap \big\{k\colon a_k(f) > 0\big\} = A_{\mathcal{P}}(f). \end{aligned}$$

It is now clear that $A \in \{K \in \mathcal{L}\colon\ K \cap \{k\colon \varphi_k \in \mathcal{P}\} = \emptyset\}$ which takes care of the first half of the proof. To conclude it, let $B \in \{K \in \mathcal{L}\colon\ K \cap \{k\colon \varphi_k \in \mathcal{P}\} = \emptyset\}$. Pick $g \in SCPD_{\mathcal{P}_1}(\Omega)$ such that $A_{\mathcal{P}_1}(g) = B$. It follows that $g \in SCPD_{\mathcal{P}}(\Omega)$. Finally,

$$\begin{aligned} B &= \{k\colon \varphi_k \notin \mathcal{P}_1\} \cap \big\{k\colon a_k(g) > 0\big\} \\ &= \big(\{k\colon \varphi_k \in \mathcal{P} \setminus \mathcal{P}_1\} \cap \big\{k\colon a_k(g) > 0\big\}\big) \cup \big(\{k\colon \varphi_k \notin \mathcal{P}\} \cap \big\{k\colon a_k(g) > 0\big\}\big) \\ &= \{k\colon \varphi_k \notin \mathcal{P}\} \cap \big\{k\colon a_k(g) > 0\big\} = A_{\mathcal{P}}(g). \end{aligned}$$

This concludes the proof. □

If $\mathcal{P} = \mathcal{P}_1$ then $\mathcal{L} = \{K \in \mathcal{L}\colon\ K \cap \{k\colon \varphi_k \in \mathcal{P}\} = \emptyset\}$ and the invariance hypothesis on $\mathcal{L}$ can be discarded.

In practice, the use of Theorem 3.4 will depend on the knowledge of a characterization of the class $SCPD_{\{0\}}(\Omega)$ and nothing else. However, even for some desirable domains Ω such characterization is not available yet. We hope this continue being a topic for future research.

In the case in which Ω is a sphere or some other similar manifolds, some subclasses of $SCPD_{\{0\}}(\Omega)$ are known. For instance, the class $\mathcal{Z}_l \cap SCPD_{\{0\}}(S^{l-1})$, in which $\mathcal{Z}_l$ stands for the bi-zonal kernels on S^{l-1}, was described in [3]. In Section 4, we prove that Theorem 3.4 can be adapted to hold for bi-zonal classes so that a characterization of $\mathcal{Z}_l \cap SCPD_{\mathcal{P}}(S^{l-1})$ can be reached. The search for versions of Theorem 3.4 for other domains and classes seems to be a problem that should deserve future attention.

4. Conditional positive definiteness on real spheres

In this section, we analyze the case in which $\Omega = S^{l-1}$, the unit sphere in $\mathbb{R}^l$. The measure ω will be the unique probability Borel measure over S^{l-1} which is $\mathcal{O}_l$-invariant, where $\mathcal{O}_l$ is the group of orthogonal transformations of $\mathbb{R}^l$. The basis $\{\varphi_k\}$ will be a basis of spherical harmonics in l dimensions. Thus, the hypothesis "$\{\varphi_k\}$ contains a basis for $\mathcal{P}$" used in previous sections is now meaningless. With this background notation established, Theorem 3.4 can be easily restated in the present case as the reader can easily verify.

Next, we discuss smaller classes of conditionally positive definite kernels on S^{l-1}. The most important ones perhaps are those composed of *bi-zonal* kernels. A kernel $f : S^{l-1} \times S^{l-1} \mapsto \mathbb{C}$ is bi-zonal when

$$f(x, y) = f(x \cdot y), \quad x, y \in S^{l-1}, \tag{4.1}$$

where $\cdot$ stands for the usual inner product of $\mathbb{R}^l$. In particular, a bi-zonal kernel f is $\mathcal{O}_l$-invariant in the following sense:

$$f\big(T(x), T(y)\big) = f(x, y), \quad x, y \in S^{l-1},\ T \in \mathcal{O}_l. \tag{4.2}$$

The symbol $\mathcal{Z}_l$ will continue standing for the set of all such kernels.

When dealing with zonal kernels, it is convenient to use spaces $\mathcal{P}$ which are $\mathcal{O}_l$-invariant in the following sense:

$$p \circ T = p, \quad p \in \mathcal{P},\ T \in \mathcal{O}_l. \tag{4.3}$$

Spherical harmonics are examples of polynomials having this property. The space $L^2(S^{l-1}, d\omega)$ also has a similar invariance property, namely,

$$\langle f \circ T, g \circ T\rangle = \langle f, g\rangle, \quad f, g \in L^2(\Omega, d\omega),\ T \in \mathcal{O}_l. \tag{4.4}$$

Lemma 4.1 below describes the $\mathcal{O}_l$-invariant spaces of spherical harmonics. The symbol $\mathcal{H}_k(S^{l-1})$ will stand for the space of spherical harmonics of degree k in l dimensions.

Lemma 4.1. *A finite-dimensional subspace of $L^2(S^{l-1}, d\omega)$ is $\mathcal{O}_l$-invariant if and only if it is a direct sum of finitely many spaces $\mathcal{H}_k(S^{l-1})$.*

Proof. See [9, p. 55], for example. □

We intend to state the results in the zonal case taking into account standard notation adopted in the literature dealing with analysis on S^{l-1} [7,16]. To do that, additional notation is needed. First, we write the orthonormal family $\{\varphi_k\}$ as a double-indexed family of the form

$$\{\varphi_k\} = \{\mathcal{F}_0, \mathcal{F}_1, \ldots\}, \tag{4.5}$$

in which

$$\mathcal{F}_k := \big\{Y^l_{kj}\colon\ j = 1, \ldots, d(k, l)\big\} \tag{4.6}$$

is a basis for $\mathcal{H}_k(S^{l-1})$. The following representation for $\mathcal{P}^l_m(S^{l-1}) := \mathcal{P}^l_m$, the space of polynomials of degree at most m in l variables, restricted to S^{l-1}, is then immediate: $\mathcal{P}^l_m(S^{l-1}) = \bigoplus_{k=0}^m \mathcal{H}_k(S^{l-1})$. The representation (1.8) takes the form

$$f(x, y) = \sum_{k=0}^{\infty} \sum_{j=1}^{d(k,l)} a_{kj}(f) Y^l_{kj}(x) \overline{Y^l_{kj}(y)}, \quad x, y \in S^{l-1}. \tag{4.7}$$

A description of $CPD_{\mathcal{P}}(S^{l-1})$ follows from Theorem 2.7. In particular, a description of $\mathcal{Z}_l \cap CPD_{\mathcal{P}}(S^{l-1})$ is easily deduced. Theorem 4.2 below is an adaptation of Theorem 3.4 to the zonal situation. We refer the reader to [7,11] for the specifics about analysis on S^{l-1}.

Theorem 4.2. *Let $\mathcal{P}$ be an $\mathcal{O}_l$-invariant m-dimensional subspace of Π and $\mathcal{P}_1$ a subspace of $\mathcal{P}$. If $\mathcal{L}$ is a translation-invariant family that represents $\mathcal{Z}_l \cap SCPD_{\mathcal{P}_1}(S^{l-1})$ then the set $\{K \in \mathcal{L}\colon\ K \cap \{k\colon\ \varphi_k \notin \mathcal{P}\} = \emptyset\}$ represents $\mathcal{Z}_l \cap SCPD_{\mathcal{P}}(S^{l-1})$.*

Proof. It suffices to adapt the proof of Theorem 3.4 to the present situation. The key step is to show that if $f \in \mathcal{Z}_l$ and $\mathcal{P}$ is $\mathcal{O}_l$-invariant then $f_{\mathcal{P}}^{\perp} \in \mathcal{Z}_l$. This can be justified along the following lines. A kernel admitting a representation as in (4.7) is bi-zonal if and only if it possesses the following additional feature:

$$a_{kj}(f) = a_{k1}(f), \quad j = 1, \ldots, d(k,l),\ k = 0, 1, \ldots. \tag{4.8}$$

Thus, if f is such a kernel and $\mathcal{P}$ is $\mathcal{O}_l$-invariant, the direct sum decomposition given in Lemma 4.1 implies that $f_{\mathcal{P}}^{\perp}$ satisfies condition (4.8). Therefore, it is bi-zonal. With this in mind, the first part of the proof goes without difficulties. The last part is handled by picking $h \in \mathcal{Z}_l \cap SCPD_{\mathcal{P}}(S^{l-1})$ from the beginning. □

We close the section looking at the special case when $\mathcal{P} = \mathcal{P}_m^l$. As we mentioned before, this is the most common choice for $\mathcal{P}$ in applications. Theorem 2.7 reads like this in this case.

Theorem 4.3. *Let f be a kernel as in* (4.7). *Then $f \in CPD_{\mathcal{P}_m^l}(S^{l-1})$ if and only if*

$$a_{kj} \geqslant 0, \quad j = 1, 2, \ldots, d(k,l),\ k = m+1, m+2, \ldots. \tag{4.9}$$

For bi-zonal kernels it takes the following aspect.

Theorem 4.4. *Let f be a kernel as in* (4.7). *Then $f \in \mathcal{Z}_l \cap CPD_{\mathcal{P}_m^l}(S^{l-1})$ if and only if*

$$a_{k1} = \cdots = a_{kd(k,l)} \geqslant 0, \quad k = m+1, m+2, \ldots. \tag{4.10}$$

The above theorem contains a description of $\mathcal{Z}_l \cap CPD_{\{0\}}(S^{l-1})$, the major result in Schoenberg's paper [15]. Due to that result, Theorem 4.4 has been quoted or used in several references (see [1,4], for example). To our knowledge, an explicit proof was missing until now.

We restate Theorem 4.2 in two steps.

Theorem 4.5. *Let f be a kernel in $CPD_{\{0\}}(S^{l-1})$. If $l \geqslant 3$, then $f \in \mathcal{Z}_l \cap SCPD_{\{0\}}(S^{l-1})$ if and only if $a_{k1} = \cdots = a_{kd(k,l)} > 0$ for infinitely many even and infinitely many odd values of k.*

Proof. See [3]. □

Theorem 4.6. *Let f be a kernel in $CPD_{\mathcal{P}_m^l}(S^{l-1})$. If $l \geqslant 3$, then $f \in \mathcal{Z}_l \cap SCPD_{\mathcal{P}_m^l}(S^{l-1})$ if and only if $a_{k1} = \cdots = a_{kd(k,l)} > 0$ for infinitely many even and infinitely many odd values of k.*

Proof. It suffices to combine Theorems 4.2 and 4.5. □

To determine an elementary description of the class $\mathcal{Z}_l \cap SCPD_{\{0\}}(S^1)$ is a question that stands for many years.

5. The case $\Omega = \Omega_{2l}$, the unit sphere in $\mathbb{C}^l$

The case $\Omega = \Omega_{2l}$, the unit sphere in $\mathbb{C}^l$, is very similar to that discussed in Section 4. Thus, we only point out what the changes are and state the results without proofs.

The group $\mathcal{O}_l$ needs to replaced with $\mathcal{U}_{2l}$, the group of all unitary transformations of $\mathbb{C}^l$. The measure ω needs to be the unique probability measure on Ω_{2l} which is $\mathcal{U}_{2l}$-invariant. Finite-dimensional $\mathcal{U}_{2l}$-invariant subspaces of $L^2(\Omega_{2l}, d\omega)$ are of the form $\bigoplus_{(r,s)\in B} \mathcal{H}_{r,s}(\Omega_{2l})$, where $B \subset \mathbb{Z}_+^2$ and $\mathcal{H}_{r,s}(\Omega_{2l})$ is the space of homogeneous $\mathbb{C}^l$-harmonic polynomials of degree m in $z \in \mathbb{C}^l$ and degree n in $\bar{z}$, restricted to Ω_{2l} (see Chapter 12 in [11]).

Since $L^2(\Omega_{2l}, d\omega) = \bigoplus_{r,s\geqslant 0} \mathcal{H}_{r,s}(\Omega_{2l})$, the basis $\{\varphi_k\}$ can be taken in the form $\bigcup_{r,s\geqslant 0} \mathcal{F}_{r,s}$, where $\mathcal{F}_{r,s} = \{Y^l_{r,s,j}\colon\ j = 1, \dots, d(r,s,l)\}$ is a basis for $\mathcal{H}_{r,s}(\Omega_{2l})$. Expression (1.8) takes the form

$$f(x,y) = \sum_{r,s=0}^{\infty} \sum_{j=1}^{d(r,s,l)} a_{r,s,j}(f) Y^l_{r,s,j}(x) \overline{Y^l_{r,s,j}(y)}, \quad x, y \in \Omega_{2l}. \tag{5.1}$$

In what follows, $P^l_{m,n} := \bigoplus_{r=0}^{m} \bigoplus_{s=0}^{n} \mathcal{H}_{r,s}(\Omega_{2l})$. Theorem 2.7 adapted to this new notation reads as follows.

Theorem 5.1. *Let f be a kernel as in* (5.1). *Then $f \in CPD_{\mathcal{P}^l_{m,n}}(\Omega_{2l})$ if and only if*

$$a_{r,s,j} \geqslant 0, \quad j = 1, \dots, d(r,s,l), \tag{5.2}$$

when either $r \geqslant m+1$ or $s \geqslant n+1$.

Bi-zonality can be easily transferred to the complex setting as the reader can easily verify. In particular, we have the following results. The symbol $\mathcal{Z}_{2l}$ will denote the class of bi-zonal kernels on Ω_{2l}.

Corollary 5.2. *Let f be a kernel as in* (5.1). *Then $f \in \mathcal{Z}_{2l} \cap CPD_{\mathcal{P}^l_{m,n}}(\Omega_{2l})$ if and only if $a_{r,s,1} = \cdots = a_{r,s,d(r,s,l)} \geqslant 0$ when either $r \geqslant m+1$ or $s \geqslant n+1$.*

Proof. It suffices to use the main theorem in [5] and Theorem 5.1. □

Theorem 5.3. *Let f be a kernel in $CPD_{\mathcal{P}^l_{m,n}}(\Omega_{2l})$. If $l \geqslant 3$, then $f \in \mathcal{Z}_{2l} \cap SCPD_{\mathcal{P}^l_{m,n}}(\Omega_{2l})$ if and only if $a_{r,s,1} = \cdots = a_{r,s,d(r,s,l)} > 0$ for infinitely many pairs (r,s) such that $r-s$ is even and infinitely many pairs (r,s) such that $r-s$ is odd.*

Proof. The condition stated in the theorem is precisely the one obtained in [6] to characterize the class $\mathcal{Z}_{2l} \cap SCPD_{\{0\}}(\Omega_{2l})$. An adaptation of Theorem 4.2 to the complex setting is all that is needed to conclude the proof. □

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