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POSITIVE DEFINITENESS: FROM SCALAR TO OPERATOR-VALUED KERNELS

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Abstract. In this paper we present a short overview of results that provide relationships among scalar, matrix-valued and certain operator-valued positive definite kernels. We refine and extend some of them in order that they may be applied for strict positive definiteness as well. This is a topic not well explored in the literature but that has potential usefulness in the characterization of several classes of positive definite and strictly positive definite kernels. This is ratified in the paper with the inclusion of a number of applications and examples.

1 Introduction

The target in this paper is to revisit several results that deal with the interrelationship among some notions of positive definiteness. After expanding some of these results in such a way that the statements cover the stronger notion of strict positive definiteness, we implement the analysis of independent applications to demonstrate the power of the results.

Positive definite kernels, also known as reproducing kernels, are functions defined on a cartesian product $X \times X$, in which X is a nonempty set, and taking values in either $\mathbb{C}$, or the space $M_p(\mathbb{C})$ of all $p \times p$ matrices with complex entries and sometimes in a space of linear operators acting on an inner product space. The famous Moore-Aronszajin Theorem ([1]) and its generalizations state that if f is positive definite kernel with domain $X \times X$, then there is a unique reproducing kernel Hilbert space associated to it and vice versa. And these Hilbert spaces can be used in a variety of instances: deformation analysis ([12]), approximation of functions ([22]), machine learning ([11]), etc. We also mention [19] for a modern analysis and a number of applications, [20] for a special treatment of vector-valued reproducing kernel Hilbert spaces and [3] for applications in probability and statistics. The theory of scalar positive definite and related kernels can be found in [2]. Here, we will focus on the kernels only making no mention to reproducing properties.

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We will close this introduction presenting two of the three definitions of (strict) positive definiteness we intend to make use of.

A matrix function $F : X \times X \to M_p(\mathbb{C})$ is said to be *a positive definite kernel* if for $n \geq 1$ and points $x_1, \ldots, x_n$ in X, the matrix $[F(x_\mu, x_\nu)]_{\mu,\nu=1}^n$ of order np is positive semi-definite, that is,

$$\sum_{\mu,\nu=1}^{n} \mathbf{c}_\mu F(x_\mu, x_\nu)\mathbf{c}_\nu^* \geq 0, \tag{1.1}$$

whenever $\mathbf{c}_1, \ldots, \mathbf{c}_n$ are (line) vectors in $\mathbb{C}^p$. As usual, the $*$ notation stands for conjugate transpose of a vector. A positive definite matrix function F is *a strictly positive definite kernel* if the matrices in the definition above are all positive definite. Thus, it requires the quadratic forms in (1.1) to be positive when the x_μ are distinct and not all the $\mathbf{c}_\mu$ are zero. The usual notion of (strict) positive definiteness of a kernel on X is recovered when we set $p = 1$ and identify $M_1(\mathbb{C})$ with $\mathbb{C}$. In particular, the quadratic forms in (1.1) take the form

$$\sum_{\mu,\nu=1}^{n} c_\mu \overline{c_\nu} F(x_\mu, x_\nu) \geq 0$$

where the c_μ are now complex numbers. The operator-valued (strictly) positive definite kernels that pertain to the scope of this paper will be introduced in Section 5.

The paper proceeds as follows. In Section 2, we discuss alternative formulations for the definition of matrix-valued (strictly) positive definite kernels. We include two examples where the usefulness of these alternative formulations is evidenced. Section 3 describes results that point how one can go from matrix-valued (strictly) positive definite kernels to scalar (strictly) positive definite kernels and vice versa, without altering the set X too much. The relevancy of results of this nature is corroborated in Section 4, where we apply the results of Section 3 in the characterization of the (strict) positive definiteness of isotropic matrix-valued kernels on the unit sphere S^d in $\mathbb{R}^{d+1}$ and of kernels on $X \times S^d$ which are isotropic with respect to the S^d component, where X is a nonempty set. In both cases, the sphere S^d can be replaced with the unit sphere in ℓ_2. Finally, in Section 5, we introduce the notion of operator-valued kernel we intend to use and establish results that allows one go from operator-valued positive definite kernels to scalar positive definite kernels and vice versa along the lines of the results described in Section 3.

2 Reformulating matrix-valued positive definiteness

The purpose of this section is to provide an equivalence for the concept of matrix-valued (strict) positive definiteness and show how it can be used in practice.

Lemma 1 is a known result in the statistical literature, a version of which appeared in [17]. Roughly speaking, it shows that one can deal with usual matrices instead of block matrices in the definition of matrix-valued positive definiteness.

Lemma 1. *Let $F : X \times X \to M_p(\mathbb{C})$ be a matrix function. The following assertions are equivalent:*

(i) *F is a positive definite kernel.*

(ii) *If n is a positive integer, $x_1, \ldots, x_n$ are points in X and $\mathbf{c}_1, \ldots, \mathbf{c}_n$ are vectors in $\mathbb{C}^p$, then the matrix $[\mathbf{c}_\mu F(x_\mu, x_\nu)\mathbf{c}_\nu^*]_{\mu,\nu=1}^n \in M_n(\mathbb{C})$ is positive semi-definite.*

Proof. If n, the x_μ and the $\mathbf{c}_\mu$ are as in (ii), then

$$\sum_{\mu,\nu=1}^{n} d_\mu \overline{d_\nu}\, \mathbf{c}_\mu F(x_\mu, x_\nu)\mathbf{c}_\nu^* = \sum_{\mu,\nu=1}^{n} (d_\mu \mathbf{c}_\mu) F(x_\mu, x_\nu)(d_\nu \mathbf{c}_\nu)^*, \tag{2.1}$$

whenever $d_1, \ldots, d_n$ are complex numbers. Thus, (i) implies (ii). If $y_1, \ldots, y_m$ are points in X and $\mathbf{d}_1, \ldots, \mathbf{d}_m$ are vectors in $\mathbb{C}^p$, then

$$\sum_{\mu,\nu=1}^{m} \mathbf{d}_\mu F(y_\mu, y_\nu)\mathbf{d}_\nu^* = \sum_{\mu,\nu=1}^{m} c_\mu \overline{c_\nu}\, \mathbf{d}_\mu F(y_\mu, y_\nu)\mathbf{d}_\nu^*,$$

where $c_\mu = 1$, $\mu = 1, \ldots, m$. Thus, (ii) implies (i). □

Proposition 2 complements Lemma 1 once it establishes a similar equivalence in the case of the strict positive definiteness.

Theorem 2. *Let $F : X \times X \to M_p(\mathbb{C})$ be a positive definite matrix function. The following assertions are equivalent:*

(i) *F is a strictly positive definite kernel.*

(ii) *If $n \geq 1$, $x_1, \ldots, x_n$ are distinct points on X and $\mathbf{c}_1, \ldots, \mathbf{c}_n$ are nonzero vectors in $\mathbb{C}^p$, then the matrix $[\mathbf{c}_\mu F(x_\mu, x_\nu)\mathbf{c}_\nu^*]_{\mu,\nu=1}^n \in M_n(\mathbb{C})$ is positive definite.*

Proof. If $d_1, \ldots, d_n$ are complex numbers not all zero and $\mathbf{c}_1, \ldots, \mathbf{c}_n$ are nonzero vectors in $\mathbb{C}^p$, then the vectors $d_1\mathbf{c}_1, \ldots, d_n\mathbf{c}_n$ are not all zero. Thus, (2.1) justifies that (i) implies (ii). Conversely, if $y_1, \ldots, y_n$ are distinct points in X and $\mathbf{d}_1, \ldots, \mathbf{d}_n$ vectors in $\mathbb{C}^p$, not all zero, then we can write

$$\mathbf{d}_\mu F(y_\mu, y_\nu)\mathbf{d}_\nu^* = (c_\mu \mathbf{c}_\mu) F(y_\mu, y_\nu)(c_\nu \mathbf{c}_\nu)^*,$$

where $\mathbf{c}_\mu = \mathbf{d}_\mu / \|\mathbf{d}_\mu\|$ and $c_\mu = \|\mathbf{d}_\mu\|$ if $\mathbf{d}_\mu \neq \mathbf{0}$ while $\mathbf{c}_\mu = (1, \ldots, p)$ and $c_\mu = 0$, otherwise. In particular, the c_μ are not all zero and the $\mathbf{c}_\mu$ are all nonzero vectors in $\mathbb{C}^p$. Thus, if (ii) holds,

$$\sum_{\mu,\nu=1}^{n} \mathbf{d}_\mu F(y_\mu, y_\nu)\mathbf{d}_\nu^* = \sum_{\mu,\nu=1}^{n} c_\mu \left[\mathbf{c}_\mu F(y_\mu, y_\nu)\mathbf{c}_\nu)^*\right] \overline{c_\nu} > 0.$$

This argument shows that F is strictly positive definite. □

Here are two examples where Lemma 1 and Theorem 2 can be applied.

Example 3. *Let H be a real inner product space of dimension at least 2 with inner product $\langle \cdot, \cdot \rangle$, S_R its unit sphere of radius R centered at 0, that is,*

$$S_R = \{v \in H : \langle v, v \rangle = R^2\},$$

and f a scalar positive definite kernel on S_R. Set $G : S_R \times S_R \to M_p(\mathbb{C})$ through the formula

$$G(x, x') = \sum_{k=0}^{\infty} A_k \langle x, x' \rangle^k, \quad x, x' \in S_R,$$

where each A_k is a positive semi-definite matrix in $M_p(\mathbb{C})$ and the series $\sum_{k=0}^{\infty} A_k R^{2k}$ is convergent. If n is a positive integer, $x_1, \ldots, x_n$ are points in S_R and $\mathbf{c}_1, \ldots, \mathbf{c}_n$ are vectors in $\mathbb{C}^p$, then

$$\left[\mathbf{c}_\mu G(x_\mu, x_\nu)\mathbf{c}_\mu^*\right]_{\mu,\nu=1}^n = \sum_{k=0}^{\infty} [\mathbf{c}_\mu A_k \mathbf{c}_\nu^*]_{\mu,\nu=1}^n \bullet \left[\langle x_\mu, x_\nu \rangle^k\right]_{\mu,\nu=1}^n,$$

where $\bullet$ stands for the Hadamard product of matrices. Hence, G is positive definite by the Schur Product Theorem ([10, P. 477]) and Lemma 1. Since

$$[\mathbf{c}_\mu f(x_\mu, x_\nu) G(x_\mu, x_\nu)\mathbf{c}_\nu^*]_{\mu,\nu=1}^n = [f(x_\mu, x_\nu)]_{\mu,\nu=1}^n \bullet [\mathbf{c}_\mu G(x_\mu, x_\nu)\mathbf{c}_\nu^*]_{\mu,\nu=1}^n,$$

a similar reasoning implies that the matrix $[\mathbf{c}_\mu f(x_\mu, x_\nu) G(x_\mu, x_\nu)\mathbf{c}_\nu^*]_{\mu,\nu=1}^n$ is positive semi-definite. These arguments along with Lemma 1 show that the kernel

$$(x, x') \in S_R \times S_R \to f(x, x')G(x, x') \tag{2.2}$$

is positive definite. We also have that

$$\mathbf{c}_\mu G(x_\mu, x_\mu)\mathbf{c}_\mu^* = \sum_{k=0}^{\infty} \mathbf{c}_\mu A_k \mathbf{c}_\mu^* \, \langle x_\mu, x_\mu \rangle^k = \sum_{k=0}^{\infty} R^{2k} \sum_{i,j=1}^{p} c_\mu^i c_\mu^j A_k^{ij}, \quad \mu = 1, \ldots, n,$$

where we are writing $\mathbf{c}_\mu = (c_\mu^1, \ldots, c_\mu^p)$ and $A_k = [A_k^{ij}]_{i,j=1}^p$. So, if the $\mathbf{c}_\mu$ are nonzero and A_k is positive definite for at least one k, then

$$\mathbf{c}_\mu G(x_\mu, x_\mu)\mathbf{c}_\mu^* > 0, \quad \mu = 1, \ldots, n,$$

that is, the entries in the main diagonal of $[\mathbf{c}_\mu G(x_\mu, x_\nu)\mathbf{c}_\nu^*]_{\mu,\nu=1}^n$ are all positive. Recalling Oppenheim's inequality ([10, P.509]), it is now promptly seen that if f is strictly positive definite, the x_μ are distinct, and A_k is positive definite for at least one k, then the matrix $[\mathbf{c}_\mu f(x_\mu, x_\nu) G(x_\mu, x_\nu)\mathbf{c}_\nu^*]_{\mu,\nu=1}^n$ is actually positive definite. Thus, by applying Theorem 2, we can see that the kernel (2.2) is strictly positive definite whenever f is so and A_k is positive definite for at least one k.

Example 4. *Let H be a (nontrivial) complex inner product space with inner product $\langle\cdot,\cdot\rangle$. According to [15], if $f : H \times H \to \mathbb{C}$ is of the form*

$$f(x,x') = \sum_{k,l=1}^{\infty} a_{k,l}\langle x,x'\rangle^k \overline{\langle x,x'\rangle}^l$$

where each $a_{k,l}$ is nonnegative and the series is convergent for all x and x', then $(x,x') \in H \times H \to f(x,x')$ is positive definite. Hence, if $G : H \times H \to M_p(\mathbb{C})$ is positive definite, Lemma 1 implies that $(x,x') \in H \times H \to f(x,x')G(x,x')$ is positive definite as well. Indeed, if n is a positive integer, $x_1,\dots,x_n$ are points in H and $\mathbf{c}_1,\dots,\mathbf{c}_n$ are vectors in $\mathbb{C}^p$, then, as before,

$$[\mathbf{c}_\mu f(x_\mu,x_\nu)G(x_\mu,x_\nu)\mathbf{c}_\nu^*]_{\mu,\nu=1}^n = [f(x_\mu,x_\nu)]_{\mu,\nu=1}^n \bullet [\mathbf{c}_\mu G(x_\mu,x_\nu)\mathbf{c}_\nu^*]_{\mu,\nu=1}^n .$$

But, the first matrix in the Hadamard product above is obviously positive semi-definite while the other one is positive semi-definite by Lemma 1. Another result in [15] reveals that $(x,x') \in H \times H \to f(x,x')$ is strictly positive definite if and only if $a_{0,0} > 0$ and $\{k-l : a_{k,l} > 0\}$ intersects every full arithmetic progression in $\mathbb{Z}$. If this is the case and $\mathbf{c}_\mu G(x_\mu,x_\mu)\mathbf{c}_\mu^* > 0$ whenever $n \geq 1$, the x_μ are distinct and the $\mathbf{c}_\mu$ are nonzero, then Oppenheim's inequality implies that $(x,x') \in H \times H \to f(x,x')G(x,x')$ is actually strictly positive definite. If G is strictly positive definite and $a_{k,l} > 0$ for just one pair (k,l), then a similar reasoning shows that $(x,x') \in (H \setminus \{0\}) \times (H \setminus \{0\}) \to f(x,x')G(x,x')$ is strictly positive definite. Implicitly, we are using the fact that if a kernel $(x,x') \in X \times X \to f(x,x') \in \mathbb{C}$ is positive definite, then so is $(y,y') \in Y \times Y \to f(y,y') \in \mathbb{C}$ for any nonempty subset Y of X.

Needless to say that Example 3 can be reformulated for spheres in complex inner product spaces while Example 4 can be adapted to hold for real inner product spaces via results described in [16]. Details will be left to the readers.

3 From matrix-valued to scalar kernels and vice-versa

No matter the setting, to characterize matrix-valued (strictly) positive definiteness is usually more difficult than to characterize its scalar cousin. In some cases, the characterizations for matrix-valued (strict) positive definiteness available in the literature either resemble or follow from the corresponding characterization in the scalar (strict) positive definiteness. In this perspective, methods that allows one to construct matrix-valued (strictly) positive definite kernels from scalar (strictly) positive definite kernels and vice versa, without the introduction of foreign players, become quite relevant. The objective in this section is to discuss some results fitting into this role.

Theorem 5 below provides a method to construct $M_p(\mathbb{C})$-valued positive definite matrix functions on a single set X from positive definite scalar kernels on the cartesian product of X with a nonempty set Y of cardinality p.

Theorem 5. *Let X be a nonempty set, $Y = \{y_1, \dots, y_p\}$ a set of cardinality p, and $f : (X \times Y)^2 \to \mathbb{C}$ a kernel. Set $F : X \times X \to M_p(\mathbb{C})$ through the formula*

$$F(x, x') = \left[f((x, y_i), (x', y_j))\right]_{i,j=1}^{p}, \quad x, x' \in X.$$

If f is a (strictly) positive definite kernel, then F is a (strictly) positive definite kernel as well.

Proof. If $x_1, \dots, x_n$ are n points in X and $\mathbf{c}_1, \dots, \mathbf{c}_n$ are vectors in $\mathbb{C}^p$, then it is easily seen that

$$\sum_{\mu,\nu=1}^{n} \mathbf{c}_\mu F(x_\mu, x_\nu) \mathbf{c}_\nu^* = \sum_{i,j=1}^{p} \sum_{\mu,\nu=1}^{n} c_\mu^i \overline{c_\nu^j} f((x_\mu, y_i), (x_\nu, y_j)),$$

in which $\mathbf{c}_\mu = (c_\mu^1, \dots, c_\mu^p)$, $\mu = 1, \dots, n$. Now observe that we can re-index the quadratic form in the right-hand side so that

$$\sum_{\mu,\nu=1}^{n} \mathbf{c}_\mu F(x_\mu, x_\nu) \mathbf{c}_\nu^* = \sum_{\alpha,\beta=1}^{np} c_\alpha \overline{c_\beta} f(z_\alpha, z_\beta),$$

where

$$c_\alpha = \begin{cases} c_1^\alpha & \text{if } \alpha \in \{1, \dots, p\} \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots & \\ c_n^{\alpha-(n-1)p} & \text{if } \alpha \in \{(n-1)p + 1, \dots, np\} \end{cases}$$

and

$$z_\alpha = \begin{cases} (x_1, y_\alpha) & \text{if } \alpha \in \{1, \dots, p\} \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots & \\ (x_n, y_{\alpha-(n-1)p}) & \text{if } \alpha \in \{(n-1)p + 1, \dots, np\}. \end{cases}$$

This is all that is needed in order to see that (i) implies (ii). Keeping the notation above, if the x_i are distinct, then so are the z_j. On the other hand, if the $\mathbf{c}_\mu$ are not all zero, then at least on c_α is nonzero. Thus, if f is strictly positive definite, then for distinct x_i and the $\mathbf{c}_\mu$ not all zero, we actually have that

$$\sum_{\mu,\nu=1}^{n} \mathbf{c}_\mu F(x_\mu, x_\nu) \mathbf{c}_\nu^* = \sum_{\alpha,\beta=1}^{np} c_\alpha \overline{c_\beta} f(z_\alpha, z_\beta) > 0.$$

This shows that F is strictly positive definite as well. □

The reader is advised that the assertion in Theorem 5 regarding the equivalence in the non strict case still holds if the y_i are not distinct. This fact justifies one implication in the following extension of Theorem 5 in which we replace the finite set Y with an arbitrary set.

Theorem 6. *Let X and Y be nonempty sets and $f : X \times Y \to \mathbb{C}$ a kernel. If X is infinite, then the following assertions are equivalent:*

(*i*) *f is positive definite.*

(*ii*) *If $p \geq 1$ and $y_1, \ldots, y_p$ are points in Y, then the matrix function $F : X \times X \to M_p(\mathbb{C})$ given by*

$$F(x, x') = \left[f((x, y_i), (x', y_j))\right]_{i,j=1}^{p}, \quad x, x' \in X.$$

is a positive definite kernel.

Proof. It suffices to prove that (*ii*) implies (*i*). Let $(x_1, y_1), \ldots, (x_m, y_m)$ be points in $X \times Y$ and $c_1, \ldots, c_m$ complex numbers. We may assume there are $p \leq m$ distinct y_j being used in this point distribution which we will call P. Since X is infinite, we may enhance P by adding additional points to it, but still using the same y_j as second components and reach, for some n, a point distribution $\{z_\alpha\}$ having the same block structure defined in the proof of Theorem 5. Finally, for $\mu \in \{1, \ldots, n\}$, we set

$$c_\mu^\alpha = \begin{cases} c_\mu & \text{if } (x_\mu, y_\alpha) \in P \\ 0 & \text{if } (x_\mu, y_\alpha) \notin P. \end{cases}$$

Under this settings, it is now clear that

$$\begin{aligned} \sum_{\alpha,\beta=1}^{np} c_\alpha \overline{c_\beta} f(z_\alpha, z_\beta) &= \sum_{i,j=1}^{p} \sum_{\mu,\nu=1}^{n} c_\mu^i \overline{c_\nu^j} f((x_\mu, y_i), (x_\nu, y_j)) \\ &= \sum_{\mu,\nu=1}^{n} \mathbf{c}_\mu F(x_\mu, x_\nu) \mathbf{c}_\nu^*, \end{aligned}$$

where $\mathbf{c}_\mu = (c_\mu^1, \ldots, c_\mu^p)$ for $\mu = 1, \ldots, n$ and F is as in (*ii*). If (*ii*) holds, we may conclude that $\sum_{\alpha,\beta=1}^{np} c_\alpha \overline{c_\beta} f(z_\alpha, z_\beta) \geq 0$. Since the c_α are arbitrary, we end up concluding that $[f(z_\alpha, z_\beta)]_{\alpha,\beta=1}^{np}$ is positive semi-definite. It follows that its principal minor $[f((x_\mu, y_\mu), (x_\nu, y_\nu))]_{\mu,\nu=1}^{m}$ is positive semi-definite as well. Thus, (*i*) holds. □

A version of Theorem 7 for strict positive definiteness is as follows. Details will be left to the readers.

Theorem 7. *Let X and Y be nonempty sets and $f : X \times Y \to \mathbb{C}$ a positive definite kernel. If X is infinite, then the following assertions are equivalent:*

(*i*) *f is strictly positive definite.*

(*ii*) *If $p \geq 1$ and $y_1, \ldots, y_p$ are distinct points in Y, then the matrix function $F : X \times X \to M_p(\mathbb{C})$ given by*

$$F(x, x') = \left[f((x, y_i), (x', y_j))\right]_{i,j=1}^{p}, \quad x, x' \in X$$

is a strictly positive definite kernel.

Next, we reverse the process and go from positive definite matrix kernels to scalar kernels.

Theorem 8. *Let* $F = [f_{ij}]_{i,j=1}^p : X \times X \to M_p(\mathbb{C})$ *be a matrix function. Define a complex function* f *on* $(X \times \{1, \dots, p\})^2$ *by the formula*

$$f((x,i),(x',j)) = f_{ij}(x,y), \quad x, x' \in X, \quad i, j \in \{1, \dots, p\}.$$

The following assertions are equivalent:

(*i*) *F is a positive definite kernel.*

(*ii*) *f is a scalar positive definite kernel.*

Proof. Let $(x_1, i_1), \dots, (x_n, i_n)$ be points in $X \times \{1, \dots, p\}$ and pick the distinct elements among the x_μ, say, $x'_1, \dots, x'_m$, $m \leq n$. It is easily seen that the $n \times n$ matrix $[f((x_j, i_j),(x_k, i_k))]_{j,k=1}^n = [f_{i_j i_k}(x_j, x_k)]_{j,k=1}^n$ is a principal minor of the $mp \times mp$ matrix $[F(x'_\mu, x'_\nu)]_{\mu,\nu=1}^m = [[f_{ij}(x'_\mu, x'_\nu)]_{i,j=1}^p]_{\mu,\nu=1}^m$. Thus, the positive semi-definiteness of the matrix $[F(x'_\mu, x'_\nu)]_{\mu,\nu=1}^m$ implies the positive semi-definiteness of the matrix $[f((x_j, i_j),(x_k, i_k))]_{j,k=1}^n$. This shows that (*i*) implies (*ii*). Conversely, if $x_1, \dots, x_m$ are points in X, $\mathbf{c}_1, \dots, \mathbf{c}_m$ are vectors in $\mathbb{C}^p$ and we write $\mathbf{c}_\mu = (c_\mu^1, \dots, c_\mu^p)$ for $\mu = 1, \dots, m$, then

$$\sum_{\mu,\nu=1}^m \mathbf{c}_\mu F(x_\mu, x_\nu)\mathbf{c}_\nu^* = \sum_{\mu,\nu=1}^m \sum_{i,j=1}^p c_\mu^i \overline{c_\nu^j} f((x_\mu, i),(x_\nu, j)).$$

Obviously, the double sum appearing above is of the form $\sum_{\alpha,\beta}^{mp} c_\alpha \overline{c_\beta} f(z_\alpha, z_\beta)$ where $z_1, \dots, z_{mp}$ are points in $X \times \{1, \dots, p\}$ and $c_1, \dots, c_{mp}$ are complex numbers. Thus, if (*ii*) holds, $\sum_{\mu,\nu=1}^m \mathbf{c}_\mu F(x_\mu, x_\nu)\mathbf{c}_\nu^* \geq 0$. Since the x_j are arbitrary, (*i*) holds as well. □

A review of the arguments employed in the proof of Theorem 8 leads to the following additional result.

Theorem 9. *Let F and f be as in Theorem 8. If F is a strictly positive definite kernel, then f is a scalar strictly positive definite kernel, and conversely.*

4 Typifying matrix-valued (strict) positive definiteness

This separated section contains applications of the results described in Section 3. As a matter of fact, the reader will notice that what is really behind the examples we have chosen is a solid method to describe matrix-valued (strictly) positive definite kernels when the scalar kernels under the same setting are known and given by special series expansions. In particular, it is reasonable to expect that results of the same nature of the ones presented here will hold in other contexts.

4.1 Kernels on $X \times S^d$

We begin with the characterization of matrix valued (strictly) positive definite kernels on $X \times S^d$ which are isotropic with respect to the spherical component. Precisely, we will provide a characterization for the positive definiteness and strict positive definiteness of a matrix kernel $F : (X \times S^d)^2 \to M_p(\mathbb{C})$ of the form

$$F((x,u),(x',v)) = f(x,y,\langle u,v\rangle), \quad x,x' \in X; u,v \in S^d,$$

in which X is a nonempty set, S^d is the unit sphere in $\mathbb{R}^{d+1}$, if $d < \infty$ and in ℓ_2 if $p = \infty$, $\langle \cdot,\cdot\rangle$ is the usual inner product in $\mathbb{R}^{d+1}$, while $f = [f_{ij}]_{i,j=1}^p : X \times X \times [-1,1] \to M_p(\mathbb{C})$ is a matrix function for which every section function $f_{ij}(x,y,\cdot)$ is continuous on $[-1,1]$.

The characterizations in the case $p = 1$ was achieved in [7], along with some other important particularities of the case. These accomplishments are outlined in Propositions 10 and 11 below. We write P_k^d to denote the Gegenbauer polynomial of degree k associated with the rational number $(d-1)/2$ if $d < \infty$ while $P_k^\infty(t) = \cos^k t$, $t \in [-1,1]$. No special normalization for them is needed. The basics on the analysis on spheres can be found in [13].

Proposition 10. *Let $f : X \times X \times [-1,1] \to \mathbb{C}$ be a function with all its section functions $f(x,y,\cdot)$ continuous on $[-1,1]$. The following assertions for the kernel F given by*

$$F((x,u),(x',v)) = f(x,x',\langle u,v\rangle), \quad x,x' \in X; u,v \in S^d,$$

are equivalent:

- *(i) F is positive definite.*
- *(ii) For each pair $(x,x') \in X \times X$ fixed, the section function $f(x,x',\cdot)$ has a series representation in the form*

$$f(x,x',s) = \sum_{k=0}^{\infty} a_k^d(x,x')P_k^d(s), \quad s \in [-1,1],$$

where $a_k^d(x,x') \in \mathbb{C}$, for $k \in \mathbb{Z}_+$ and $x,x' \in X$, each kernel $(x,x') \in X \times X \mapsto a_k^d(x,x')$ is positive definite and $\sum_{k=0}^{\infty} a_k^d(x,x)P_k^d(1) < \infty$, for all $x \in X$.

Proposition 11. *Under the assumptions and notation in Proposition 10, assume F is positive definite. If $d \geq 2$, then the following assertions are equivalent:*

- *(i) F is strictly positive definite.*
- *(ii) If m is a positive integer, $x_1,\dots,x_m$ are distinct points in X, and $\mathbf{c}$ is a vector in $\mathbb{C}^m$, then the set*

$$\left\{k \in \mathbb{Z}_+ : \mathbf{c}\left[a_k^d(x_\mu,x_\nu)\right]_{\mu,\nu=1}^m \mathbf{c}^* > 0\right\}$$

contains infinitely many even and infinitely many odd integers.

(*iii*) *If m is a nonnegative integer, then the kernels*

$$(x,x') \in X \times X \mapsto \sum_{k\geq m} a^d_{2k+1}(x,x') \quad \text{and} \quad (x,x') \in X \times X \mapsto \sum_{k\geq m} a^d_{2k}(x,x')$$

are strictly positive definite.

The following lemma provides simple examples of matrix-valued positive definite kernels on $X \times S^d$.

Lemma 12. *Let $h : X \times X \to M_p(\mathbb{C})$ be a positive definite kernel. If $k \in \mathbb{Z}_+$, then the matrix function $((x,u),(x',v)) \in (X \times S^d)^2 \mapsto f(x,x',\langle u,v\rangle)$ in which*

$$f(x,x',s) = h(x,y)P^d_k(s), \quad x,x' \in X; s \in [-1,1],$$

is a positive definite kernel.

Proof. We sketch the proof in the case $p < \infty$ only. The addition theorem for spherical harmonics asserts the existence of a positive constant $C = C(k,d) > 0$ such that

$$CP^d_k(u,\cdot v) = \sum_{\alpha=1}^{\delta} S^d_{k,\alpha}(u)\overline{S^d_{k,\alpha}(v)}, \quad u,v \in S^d,$$

in which $\delta = \delta(k,d)$ is the dimension of the space of all spherical harmonics of degree k in $d+1$ dimensions while $\{S^d_{k,1},\ldots,S^d_{k,\delta}\}$ is an orthonormal basis of the same space with respect to the usual inner product of the space $L^2(S^d)$ (see [13, P.19] for details). Looking at the quadratic form pertaining to the definition of positive definiteness, we can see that

$$C\sum_{\mu,\nu=1}^{n} \mathbf{c}_\mu f(x_\mu,y_\nu,\langle u_\mu,u_\mu\rangle)\mathbf{c}^*_\nu = \sum_{\alpha=1}^{\delta}\sum_{\mu,\nu=1}^{n} \left(S^d_{k,\alpha}(u_\mu)\mathbf{c}_\mu\right) h(x_\mu,y_\nu) \left(S^d_{k,\alpha}(u_\nu)\mathbf{c}_\nu\right)^*.$$

The positive definiteness of $h : X \times X \to M_p(\mathbb{C})$ reveals that the last expression above is nonnegative. □

As an application of Theorems 5 and 8 we now prove a matrix version of Theorem 10.

Theorem 13. *Let $f = [f_{ij}] : X \times X \times [-1,1] \to M_p(\mathbb{C})$ be a matrix function. Assume all the section functions $f_{ij}(x,x',\cdot)$ are continuous on $[-1,1]$. The following assertions are equivalent:*

(*i*) *The kernel $F : (X \times S^d)^2 \to M_p(\mathbb{C})$ given by*

$$F((x,u),(x',v)) = f(x,x',\langle u,v\rangle), \quad x,x' \in X; u,v \in S^d,$$

is positive definite.

(*ii*) *For each pair* $(x, x') \in X^2$*, the section function* $f(x, x', \cdot)$ *has a matrix representation in the form*

$$f(x, x', s) = \sum_{k=0}^{\infty} A_k^d(x, x') P_k^d(s), \quad s \in [-1, 1],$$

where $A_k^d(x, x') \in M_p(\mathbb{C})$*,* $x, x' \in X$*, every kernel* $(x, x') \in X^2 \mapsto A_k^d(x, x') \in M_p(\mathbb{C})$ *is positive definite, and* $\sum_{k=0}^{\infty} A_k^d(x, x) P_k^d(1) < \infty$ *for all* $x \in X$*.*

Proof. Lemma 12 along with the fact that positive definiteness is preserved under pointwise limits show that (ii) implies (i). In order to prove (i) implies (ii), we will apply Theorem 8. If F is positive definite, then the theorem asserts that the formula

$$g(((x, u), i), ((x', v), j)) = f_{ij}(x, x', \langle u, v \rangle), \quad x, x' \in X; u, v \in S^d; 1 \leq i, j \leq p,$$

defines a positive definite kernel $g : [(X \times S^d) \times \{1, \ldots, p\}]^2 \to \mathbb{C}$. Equivalently, the formula

$$h((x, i), u)), (x', j), v))) = f_{ij}(x, x', \langle u, v \rangle), \quad x, x' \in X; 1 \leq i, j \leq p; u, v \in S^d,$$

defines a positive definite kernel $h : [(X \times \{1, \ldots, l\})]^2 \times S^d \to \mathbb{C}$. Reporting to Theorem 10, we can infer that for each pair $((x, i), (x', j)) \in (X \times \{1, \ldots, l\})^2$, the section function $f_{ij}(x, x', \cdot)$ has a series representation in the form

$$f_{ij}(x, x', s) = \sum_{k=0}^{\infty} a_k^d((x, i), (x', j)) P_k^d(s), \quad s \in [-1, 1],$$

in which all the coefficients $a_k^d((x, i), (x', j))$ are complex numbers, every kernel

$$((x, i), (x', j) \in (X \times \{1, 2, \ldots, l\})^2 \mapsto a_k^d((x, i), (x', j))$$

is positive definite, and

$$\sum_{k=0}^{\infty} a_k^d((x, i), (x, i)) P_k^d(1) < \infty, \tag{4.1}$$

for all $(x, i) \in X \times \{1, \ldots, p\}$. It is now clear that

$$f(x, x', s) = \sum_{k=0}^{\infty} A_k^d(x, x') P_k^d(s), \quad x, x' \in X, \quad s \in [-1, 1],$$

in which

$$A_k^d(x, x') = \left[a_k^d((x, i), (x', j)) \right]_{i,j=1}^{p}, \quad x, x' \in X.$$

Theorem 5 asserts the positive definiteness of the matrix function $(x, y) \in X^2 \to A_k^d(x, x') \in M_p(\mathbb{C})$ while the convergence of $\sum_{k=0}^{\infty} A_k^d(x, x) P_k(1)$ for all $x \in X$ follows from (4.1). Thus, (ii) holds. □

In Theorem 14 we go one step further and derive a characterization for strict positive definiteness in the setting of Theorem 13 but restricted to the case $d > 1$.

Theorem 14. $(d \geq 2)$ *Let* $f = [f_{ij}] : X \times X \times [-1,1] \to M_p(\mathbb{C})$ *be a matrix function. Assume all the section functions* $f_{ij}(x, x', \cdot)$ *are continuous on* $[-1,1]$ *and that the matrix function* $F : (X \times S^d)^2 \to M_p(\mathbb{C})$ *given by*

$$F((x,u),(x',v)) = f(x,x',\langle u,v\rangle), \quad x,x' \in X; u,v \in S^d,$$

is positive definite. The following assertions are equivalent:
(i) The kernel F *is strictly positive definite;*
(ii) For every nonnegative integer m*, the matrix kernels*

$$(x,x') \in X \times X \mapsto \sum_{k \geq m} A^d_{2k+1}(x,x'), \ \sum_{k \geq m} A^d_{2k}(x,x')$$

are strictly positive definite.

Proof. If F is strictly positive definite, then Theorem 9 reveals that the formula

$$g(((x,i),u),((x',j),v)) = f_{ij}(x,x',\langle u,v\rangle), \quad x,x' \in X; u,v \in S^d; 1 \leq i,j \leq p,$$

defines a strictly positive definite kernel $g : [(X \times \{1,\ldots,p\}) \times S^d]^2 \to \mathbb{C}$. By Theorem 10, we can write

$$f_{ij}(x,x',s) = \sum_{k=0}^{\infty} b^d_k((x,i),(x',j)) P^d_k(s), \quad s \in [-1,1]; x,x' \in X; 1 \leq i,j \leq p,$$

where $b^d_k((x,i),(x',j)) \in \mathbb{C}$, $k \in \mathbb{Z}_+$, $x,x' \in X$, each kernel $((x,i),(x',j)) \in X \times X \mapsto b^d_k((x,i),(x',j))$ is positive definite, $\sum_{k=0}^{\infty} b^d_k((x,i),(x,i)) P^d_k(1) < \infty$, for $(x,i) \in X \times \{1,\ldots,p\}$, and for each nonnegative integer m, the kernels

$$((x,i),(x',j)) \in (X \times \{1,\ldots,p\})^2 \mapsto \sum_{k \geq m} b^d_{2k+1}((x,i),(x',j))$$

and

$$((x,i),(x',j)) \in (X \times \{1,2,\ldots,p\})^2 \mapsto \sum_{k \geq m} b^d_{2k}((x,i),(x',j))$$

are strictly positive definite. However, Theorem 5 implies that, for each $m \geq 0$, the matrix functions

$$(x,x') \in X^2 \to \sum_{k \geq m} [b^d_{2k+1}((x,i),(x',j))]^p_{i,j=1}$$

and

$$(x,x') \in X^2 \to \sum_{k \geq m} [b^d_{2k}((x,i),(x',j))]^p_{i,j=1}$$

define, likewise, strictly positive definite kernels. In order to see that (ii) holds, it suffices to observe that

$$\begin{aligned}[f_{ij}(x,x',s]_{i,j=1}^p &= \left[\sum_{k=0}^{\infty} b_k^d((x,i),(x',j))P_k^d(s)\right]_{i,j=1}^p \\ &= \sum_{k=0}^{\infty}\left[b_k^d((x,i),(x',j))\right]_{i,j=1}^p P_k^d(s), \qquad x,y\in X.\end{aligned}$$

which implies, by uniqueness, that

$$A_k^d(x,x') = [b_k^d((x,i),(x',j))]_{i,j=1}^p, \quad k\geq 0, \quad x,x'\in X. \tag{4.2}$$

Thus (i) implies (ii). Conversely, keeping the notation in (4.2), if (ii) holds, Theorem 9 reveals that, for every $m\geq 0$, $g,h:(X\times\{1,\ldots,p\})^2\to\mathbb{C}$ given by

$$g((x,i),(x',j)) = \sum_{k\geq m} b_{2k+1}^d((x,i),(x',j)), \quad x,x'\in X; i,j\in\{1,\ldots,p\},$$

and

$$h((x,i),(x',j)) = \sum_{k\geq m} b_{2k}^d((x,i),(x',j)), \quad x,x'\in X; i,j\in\{1,\ldots,p\},$$

are strictly positive definite kernels. An application of Theorem 11 now shows that the kernel $G:[(X\times\{1,\ldots,p\})\times S^d]^2\to\mathbb{C}$ given by the formula

$$H(((x,i),u),((x',j),v)) = \sum_{k=0}^{\infty} b_k^d((x,i),(x',j))P_k^d(\langle u,v\rangle)$$

is strictly positive definite. Equivalently, $H:[(X\times S^d)\times\{1,\ldots,p\}]^2\to\mathbb{C}$ given by

$$H(((x,u),i),((x',v),j)) = \sum_{k=0}^{\infty} b_k^d((x,i),(x',j))P_k^d(\langle u,v\rangle)$$

is strictly positive definite. Finally, Theorem 5 implies that the matrix function

$$((x,u),(x',v))\in(X\times S^d)^2\to\left[\sum_{k=0}^{\infty} b_k^d((x,i),(x',j))P_k^d(\langle u,v\rangle)\right]_{i,j=1}^p$$

is strictly positive definite as well. However, this matrix function is nothing but F. Therefore, (i) holds. □

4.2 Kernels on S^d

Here, we will consider isotropic matrix functions of the form $F = [f_{ij}]_{i,j=1}^p : S^d \times S^d \to M_p(\mathbb{C})$, where $d \geq 2$ and each f_{ij} is continuous. As before, isotropy of F will mean that

$$F(x,y) = f(\langle x, y\rangle), \quad x, y \in S^d,$$

for some function $f : [-1,1] \to \mathbb{C}$. We will recover the characterization for the strict positive definiteness of continuous matrix functions on S^d obtained in [8], as an application of the results in Section 3 and Subsection 4.1.

According to either Hannan ([9, p.102]) or Yaglom ([21, p.387]), a continuous and isotropic kernel $F : S^d \times S^d \to M_p(\mathbb{C})$ is positive definite if and only if the isotropic part f of F is a matrix function possessing a convergent series representation in the form

$$f(s) = \sum_{k=0}^{\infty} A_k P_k^d(s), \quad s \in [-1,1], \tag{4.3}$$

in which each A_k is a nonnegative definite element of $M_p(\mathbb{C})$. If $A_k = [A_k^{ij}]$, convergence of the series above means that

$$\sum_{i=0}^{\infty} A_k^{ij} P_k^d(1) < \infty, \quad i, j = 1, \ldots, p.$$

We observe that for a positive definite kernel F as above, the entries f_{ii} are real-valued functions.

If a kernel F as above is strictly positive definite, then Theorem 8 implies that the kernel $g : (S^d \times \{1,\ldots,p\})^2 \to \mathbb{C}$ given by

$$g((u,i),(v,j)) = \sum_{k=0}^{\infty} A_k^{ij} P_k^d(\langle u, v\rangle), \quad u, v \in S^d; i, j \in \{1,\ldots,p\},$$

is strictly positive definite. Equivalently, $h : (\{1,\ldots,p\} \times S^d)^2 \to \mathbb{C}$ given by

$$h((i,u),(j,v)) = \sum_{k=0}^{\infty} A_k^{ij} P_k^d(\langle u, v\rangle), \quad i, j \in \{1,\ldots,p\}; u, v \in S^d,$$

is strictly positive definite. Since this representation fits into that in Theorem 10 with $X = \{1,\ldots,p\}$, we know already that each kernel

$$(i,j) \in \{1,\ldots,p\}^2 \to A_k^{ij}$$

is positive definite. Theorem 11 reveals that the set

$$\left\{ k \in \mathbb{Z}_+ : \mathbf{c} \left[A_k^{i(\mu)i(\nu)} \right]_{\mu,\nu=1}^m \mathbf{c}^* > 0 \right\}$$

contains infinitely many even and infinitely many odd integers, whenever $m \leq p$, $i(1), \ldots, i(m)$ are distinct elements of $\{1, \ldots, p\}$ and $\mathbf{c}$ is a nonzero vector in $\mathbb{C}^m$. However, this is equivalent to saying that

$$\{k \in \mathbb{Z}_+ : \mathbf{c}A_k\mathbf{c}^* > 0\}$$

contains infinitely many even and infinitely many odd integers when $\mathbf{c} \in \mathbb{C}^p \setminus \{0\}$. This process is reversible along the same lines. Therefore, we have recovered the following result.

Theorem 15. $(d \geq 2)$ *Let* $F = [f_{ij}]_{i,j=1}^p : S^d \times S^d \to M_p(\mathbb{C})$ *be an isotropic matrix function with each* f_{ij} *continuous. If* F *is positive definite with series representation implied by* (4.3)*, then the following assertions are equivalent:*

(*i*) *F is strictly positive definite;*

(*ii*) *If* $\mathbf{c}$ *is a nonzero vector in* $\mathbb{C}^p$*, then the set*

$$\{k \in \mathbb{Z}_+ : \mathbf{c}A_k\mathbf{c}^* > 0\}$$

contains infinitely many even and infinitely many odd integers.

As far as we know, versions of Theorems 14 and 15 remain elusive in the case in which the sphere S^d is replaced with S^1.

5 From operator-valued to scalar kernels and vice-versa

In this section, we go one step further, and establish a connection between operator-valued (strictly) positive definite kernels and scalar (strictly) positive definite kernels. The notions of operator-valued kernels we are interested in are as follows.

Let $(H, \langle \cdot, \cdot \rangle)$ be an inner product space and write $\mathcal{L}(H)$ to denote the space of all linear operators on H. The action of an operator $T \in \mathcal{L}(H)$ on a vector $v \in H$ will be written Tv. A kernel $F : X \times X \to \mathcal{L}(H)$ is *positive definite* if

$$\sum_{\mu,\nu=1}^{n} \langle F(x_\mu, x_\nu)v_\mu, v_\nu \rangle \geq 0, \tag{5.1}$$

whenever $n \geq 1$, $x_1, \ldots, x_n$ are distinct points in X and $v_1, \ldots, v_n$ are vectors in H. A positive definite kernel $F : X \times X \to \mathcal{L}(H)$ is *strictly positive definite* if the inequalities above are strict when the v_μ are nonzero. In applications, the definitions above may demand additional requirements: $\mathcal{L}(H)$ can be replaced with $\mathcal{B}(H)$, i.e., the set of all continuous operators on H while the kernel F may be assumed to be continuous with respect to the operator norm on $\mathcal{B}(H)$. Another common requirement is $F(x, x') = F(x', x)^*$, $x, x' \in X$, where $*$ stands for the adjoint operator. For instance, these adjustments are frequently found in some settings of learning theory as the reader can verify in [4, 18, 23] and some references therein.

Here are some simple examples of operator-valued positive definite kernels. If $P : H \to H$ is a linear *positive operator* in the sense that $\langle P(v), v\rangle \geq 0$, $v \in H$, and $f : X \times X \to \mathbb{C}$ is a positive definite kernel, then $F : X \times X \to \mathcal{L}(H)$ given by

$$F(x, x') = f(x, x')P, \quad x, x' \in X,$$

is positive definite. Indeed, for points $x_1, \ldots, x_n$ in X and vectors $v_1, \ldots, v_n$ in H,

$$[\langle F(x_\mu, x_\nu)v_\mu, v_\nu\rangle]_{\mu,\nu=1}^n = [f(x_\mu, x_\nu)]_{\mu,\nu=1}^n \bullet [\langle Pv_\mu, v_\nu\rangle)]_{\mu,\nu=1}^n,$$

and the matrix $[\langle F(x_\mu, x_\nu)v_\mu, v_\nu\rangle]_{\mu,\nu=1}^n$ is then positive semi-definite. In particular, (5.1) holds. Further, if f is strictly positive definite and P is *positive definite* in the sense $\langle P(v), v\rangle > 0$, $v \in H \setminus \{0\}$, then F is actually strictly positive definite. To see that one needs to invoke Oppenheim's inequality. A similar reasoning shows that if $f : X \times X \to \mathbb{C}$ is a positive definite kernel and $G : X \times X \to \mathcal{L}(H)$ is positive definite, then $H : X \times X \to \mathcal{L}(H)$ given by

$$H(x, x') = f(x, x')G(x, x'), \quad x, x' \in X,$$

is positive definite as well. If both f and G are strictly positive definite, then the same is true of H. Finally, let $T : H_1 \to H_2$ be a linear transformation between complex inner product spaces. If $F : X \times X \to \mathcal{L}(H_1)$ is positive definite, then $G : X \times X \to \mathcal{L}(H_2)$ given by $G(x, x') = T \circ F(x, x') \circ T^*$, $x, x' \in X$, is positive definite too. Further, if F is strictly positive definite and T is invertible, then F is strictly positive definite.

We will make use of the following technical lemma, the proof of which is left to the readers.

Lemma 16. *Let X and Y be nonempty sets and $f : X \times Y \to \mathbb{C}$ a kernel. The following assertions are equivalent:*

(i) *f is (strictly) positive definite.*

(ii) *If $x_1, \ldots, x_m$ are distinct points in X and $y_1, \ldots, y_n$ are (distinct) points in Y, then the matrix $[f((x_\mu, y_i), (x_\nu, y_j))]_{i,j=1}^n]_{\mu,\nu=1}^m$ is positive semi-definite (definite).*

Theorem 17 below provides a simple method to produce scalar kernels from operator-valued kernels. The only additional requirement needed is the use of a fixed Hamel basis $\{u_r : r \in J\}$ of H.

Theorem 17. *Let $F : X \times X \to \mathcal{L}(H)$ be an operator-valued kernel. Define $f : (X \times J)^2 \to \mathbb{C}$ by the formula*

$$f((x, r), (y, s)) = \langle F(x, y)u_s, u_r\rangle, \quad x, y \in X; r, s \in J.$$

If F is (strictly) positive definite, then so is f.

Proof. Let $x_1, \dots, x_m$ be distinct points in X and $r_1, \dots, r_n$ distinct points in J. For complex numbers $c_{\mu,i}$, $\mu = 1, \dots, m$, $i = 1, \dots, n$, set

$$v_\mu = \sum_{i=1}^{n} c_{\mu,i} u_{r_i}, \quad \mu = 1, \dots, m.$$

If F is positive definite, then we have that

$$\sum_{\mu,\nu=1}^{m} \sum_{i,j=1}^{n} c_{\mu,i} \overline{c_{\nu,j}} f((x_\mu, r_i), (x_\nu, r_j)) = \sum_{\mu,\nu=1}^{m} \langle F(x_\mu, x_\nu) v_\mu, v_\nu \rangle \geq 0,$$

and the matrix $[f((x_\mu, r_i), (x_\nu, r_j))]_{i,j=1^n}]_{\mu,\nu=1}^{m}$ is positive semi-definite. By Lemma 16, f must be positive definite. Further, if the $c_{\mu,i}$ are nonzero, then the fact that $\{u_r : r \in J\}$ is a basis of H shows that the v_μ are nonzero vectors. Thus, if F is strictly positive definite, then the inequality above is actually strict. The same Lemma 16 now implies that f is strictly positive definite. □

Needless to say that Theorem 17 holds with the same proof for operator-valued kernels of the form $F : X \times X \to \mathcal{B}(H)$.

Next, we present a procedure that allows one to go from scalar positive definite kernels on $X \times J$ to operator-valued kernels. For a fixed kernel $f : (X \times J)^2 \to \mathbb{C}$ we will make use of the quadratic form $Q : (X \times H)^2 \to \mathbb{C}$ given by

$$Q((x, u), (x', v)) = \sum_i \sum_j a_i \overline{b_j} f((x, r_i), (x', r_j)), \quad x, x' \in X; u, v \in H,$$

in which $u = \sum_i a_i u_{r_i}$ and $v = \sum_j b_j u_{s_j}$ (both sums are finite).

Theorem 18. *Let $f : (X \times J)^2 \to \mathbb{C}$ be a kernel and assume that*

$$Q((x, u), (x', v)) = \langle F(x, x') u, v \rangle, \quad x, x' \in X; u, v \in H,$$

in which $F : X \times X \to \mathcal{L}(H)$. If f is (strictly) positive definite, then so is F.

Proof. Let $x_1, \dots, x_n$ be distinct elements of X and $v_1, \dots, v_n$ vectors in H. If we write $v_\mu = \sum_{i=1}^{m} c_{\mu,i} u_{r_i}, \mu = 1, \dots, n$, where $r_1, \dots, r_m$ are distinct points in J and the $c_{\mu,i}$ are complex numbers, then

$$\sum_{\mu,\nu=1}^{n} \langle F(x_\mu, x_\nu) v_\mu, v_\nu \rangle = \sum_{\mu,\nu=1}^{n} \sum_{i,j=1}^{m} c_{\mu,i} \overline{c_{\nu,j}} f((x_\mu, r_i), (x_\nu, r_j)).$$

If f is positive definite, then an application of Lemma 16 implies that the matrix $[f((x_\mu, r_i), (x_\nu, r_j))]_{i,j=1}^{m}]_{\mu,\nu=1}^{n}$ is positive semi-definite. Thus, F is positive definite. If f is strictly positive definite, then the same Lemma 16 implies that the matrix $[f((x_\mu, r_i), (x_\nu, r_j))]_{i,j=1}^{m}]_{\mu,\nu=1}^{n}$ is positive definite. Now, if the vectors v_μ are nonzero, then not all the complex numbers $c_{\mu,i}$ will be zero, and therefore the previous inequality will be strict. Thus, F is strictly positive definite as well. □

The following piece of information may be useful if one intends to deal with operator-valued kernels of the form $F : X \times X \to \mathcal{B}(H)$: if $F : X \times X \to \mathcal{L}(H)$ is positive definite and $F(x, x)$ belongs to $\mathcal{B}(H)$ for all $x \in X$, then all the $F(x, x')$ will belong to $\mathcal{B}(H)$. Indeed, the positive definiteness of F implies that

$$\begin{bmatrix} \langle F(x,x)u,u\rangle & \langle F(x,x')u,v\rangle \\ \langle F(x',x)v,u\rangle & \langle F(x',x')v,v\rangle \end{bmatrix}$$

is positive semi-definite, whenever $x, x' \in X$ and $u, v \in H$. In particular,

$$\left|\langle F(x,x')u,v\rangle\right|^2 \leq \langle F(x,x)u,u\rangle\langle F(x',x')v,v\rangle, \quad x,x' \in X; u,v \in H.$$

However, if each $F(x, x)$ belongs to $\mathcal{B}(H)$, we can find positive constants M_x and $M_{x'}$ so that

$$\left|\langle F(x,x')u,v\rangle\right|^2 \leq M_x M_{x'} \langle u,u\rangle\langle v,v\rangle, \quad x,x' \in X; u,v \in H.$$

This implies that

$$\langle F(x,x')(u), F(x,x')(u)\rangle \leq \sqrt{M_x M_{x'}}\, \langle u,u\rangle, \quad x,x' \in X; u \in H.$$

that is, $F(x, x')$ belongs to $\mathcal{B}(H)$.

The literature lacks of consistent applications involving the results described in this section. Applications aligned with those described in Section 4 can not implemented because characterizations of operator-valued strictly positive definite kernels are rare in the literature. In any case, here are two results that resemble Theorems 17 and 18, for special choices of X and F.

Example 19. *Let $X = \mathbb{R}^m$ and assume that H is a separable Hilbert space. If $F : X \to \mathcal{B}(H)$ is ultraweakly continuous, then the operator valued kernel*

$$(x, x') \in X \times X \mapsto F(x - y) \in \mathcal{B}(H)$$

is positive definite if and only if the kernels

$$(x, x') \in X \times X \mapsto \langle F(x - y)u, u\rangle, \quad u \in H,$$

are positive definite. This fact is implied by results proved in [14].

Example 20. *Let H be a separable Hilbert space and $F : [0, \infty) \to \mathcal{B}(H)$ a ultraweakly continuous function for which $F(0)$ is trace-class. If the kernels*

$$(x, x') \in \mathbb{R}^m \times \mathbb{R}^m \mapsto \langle F(\|x - x'\|)u, u\rangle, \quad m \in \mathbb{Z}_+; u \in H,$$

are all positive definite, in which $\|\cdot\|$ denotes the usual norm in $\mathbb{R}^m$, then each operator-valued kernel

$$(x, x') \in \mathbb{R}^m \times \mathbb{R}^m \mapsto F(\|x - x'\|)$$

is positive definite. Further, each kernel above is strictly positive definite if and only if the functions

$$t \in [0, \infty) \mapsto \langle F(t)u, u \rangle, \quad u \in H \setminus \{0\},$$

are nonconstant. The proof of this result appeared in the recent paper [6]. It is worth mentioning that [6] an impressive source of results resembling Theorems 17 and 18 in many aspects.

We would like to point out that some of the results proved in this work were motivated by others considered in J. C. Guella's dissertation ([5]) concluded in 2019 at ICMC-Universidade de São Paulo, under my sypervision.

References

[1] N. Aronszajin, *Theory of reproducing kernels*, Trans. Amer. Math. Soc. **68**(1950), 337-404. MR51437 Zbl 0037.20701.

[2] C. Berg, J. P. R. Christensen, and P. Ressel, *Harmonic analysis on semigroups. Theory of positive definite and related functions*, Graduate Texts in Mathematics, 100, Springer-Verlag, New York, 1984. MR747302 Zbl 0619.43001.

[3] A. Berlinet and C. Thomas-Agnan, *Reproducing kernel Hilbert spaces in probability and statistics*, With a preface by Persi Diaconis, Kluwer Academic Publishers, Boston, 2004. MR2239907 Zbl 1145.62002.

[4] M. Brault, M. Hainonen, and F. d'Alché-Buc, *Random Fourier features for operator-valued kernels*, JMLR: Workshop and Conference Proceedings 63:110-125, 2016.

[5] J. C. Guella, *A unifying approach to isotropic and radial positive definite kernels*, Dissertation, ICMC-Universidade de São Paulo, 2019.

[6] J. Guella, *Operator valued positive definite kernels and differentiable universality*, arXiv:2003.11199v1 [math.FA], 2020.

[7] J. C. Guella and V. A. Menegatto, *Schoenberg's Theorem for positive definite functions on products: A unifying framework*, J. Fourier Anal. Appl. **25** (2019), no. 4, 1424-1446. MR3977123 Zbl 1420.42005.

[8] J. C. Guella, V. A. Menegatto, and E. Porcu, *Strictly positive definite multivariate covariance functions on spheres*, J. Multivariate Anal., **166** (2018), 150-159. MR3799640 Zbl 06869756.

[9] E. J. Hannan, *Multiple time series*, John Wiley and Sons, Inc., New York-London-Sydney, 1970. MR279952 Zbl 0211.49804.

[10] R. A. Horn and C. R. Johnson, *Matrix analysis*, Second edition, Cambridge University Press, Cambridge, 2013. MR2978290 Zbl 1267.15001.

[11] C. A. Micchelli and M. Pontil, *On learning vector-valued functions*, Neural Computation **17** (2005), 177- 204. MR2175914 Zbl 1092.93045.

[12] M. Micheli and J. A. Glaunc, *Matrix-valued kernels for shape deformation analysis*, Geometry, Imaging and Computing **1** (2014), no. 1, 57-139. MR3392140 Zbl 1396.46025.

[13] C. Müller, *Analysis of spherical symmetries in Euclidean spaces*, Applied Mathematical Sciences, 129. Springer-Verlag, New York, 1998. MR1483320 Zbl 0884.33001.

[14] K.-H. Neeb, *Operator-valued positive definite kernels on tubes*, Monatsh. Math. **126**(2) (1998), 125-160. MR1639387 Zbl 1074.43004.

[15] A. Pinkus, *Strictly Hermitian positive definite functions*, J. Anal. Math. **94** (2004), 293-318. MR2124464 Zbl 1074.43004.

[16] A. Pinkus, *Strictly positive definite functions on a real inner product space*, Adv. Comput. Math. **20** (2004), no. 4, 263-271. MR2032278 Zbl 1142.42307.

[17] E. Porcu and V. Zastavnyi, *Characterization theorems for some classes of covariance functions associated to vector valued random fields*, J. Multivariate Anal., **102** (2011), no. 9, 1293-1301. MR2811618 Zbl 1219.60053.

[18] A. Saha and P. Balamurugan, *Learning with operator-valued kernels in reproducing kernel Krein spaces*, in Advances in Neural Information Processing Systems 33 (NeurIPS 2020). Edited by: H. Larochelle, M. Ranzato, R. Hadsell, M.F. Balcan, and H. Lin., 11 pp.

[19] S. Saitoh and Y. Sawano, *Theory of reproducing kernels and applications*, Developments in Mathematics, 44. Springer, Singapore, 2016. MR3560890 Zbl 1358.46004.

[20] L. Schwartz, *Sous-espaces hilbertiens d'espaces vectoriels topologiques et noyaux associés (noyaux reproduisants)*, J. Anal. Math. **13** (1964), 115-256. MR179587 Zbl 0124.06504.

[21] A. M. Yaglom, *Correlation theory of stationary and related random functions, Vol. I, Basic results*, Springer Series in Statistics, Springer-Verlag, New York, 1987. MR893393 Zbl 0685.62077.

[22] D. Wittwar, G. Santin, and B. Haasdonk, *Interpolation with uncoupled separable matrix-valued kernels*. Dolomites Res. Notes Approx. **11** (2018), 23-29. MR3895571.

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[23] Haizhang Zhang, Yuesheng Xu, and Qinghui Zhang, *Refinement of operator-valued reproducing kernels*, J. Mach. Learn. Res., **13** (2012), 91-136. MR2913695 Zbl 1283.68310.

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