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MATRIX–VALUED POSITIVE DEFINITE KERNELS GIVEN BY EXPANSIONS: STRICT POSITIVE DEFINITENESS

W. FRANCA AND V. A. MENEGATTO*

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Abstract. Matrix functions of the form $(x,y) \in \Omega \times \Omega \mapsto \sum_\alpha A_\alpha f_\alpha(x,y)$, in which Ω is a nonempty set, the A_α are positive semi-definite matrices of the same fixed order, the f_α are complex-valued positive definite kernels on Ω, and the series is convergent for all x and y in Ω define matrix-valued positive definite kernels on Ω. Here, the sum may be multi-indexed, Ω may be endowed with either a topological or a metric structure, and $\{f_\alpha\}$ may inherit properties attached to the setting. In this paper, we present a criterion that establishes an abstract necessary and sufficient condition in order that the kernel is strictly positive definite on Ω. We point some implications and connections of the criterion in some relevant and concrete settings in order to motivate future work on the topic.

1. Introduction

This paper is mainly concerned with matrix functions that define matrix-valued positive definite kernels on a nonempty set Ω. If we write $M_p(\mathbb{C})$ to denote the set of all complex matrices of order p, a matrix-valued kernel $F : \Omega \times \Omega \to M_p(\mathbb{C})$ is said to be *positive definite* on Ω if for $n \geqslant 1$ (but at most the cardinality $|\Omega|$ of Ω) and points $x_1, \ldots, x_n$ in Ω, the matrix $[F(x_i,x_j)]_{i,j=1}^n$ of order np is positive semi-definite, that is,

$$\sum_{i,j=1}^{n} \mathbf{c}_i^* F(x_i,x_j)\mathbf{c}_j \geqslant 0, \tag{1}$$

when $\mathbf{c}_1, \ldots, \mathbf{c}_n$ are (column) vectors in $\mathbb{C}^p$ while the star notation refers to the conjugate transposition of vectors. A positive definite matrix-valued kernel F is *strictly positive definite* on Ω if the matrices in the definition above are all positive definite when the x_i are distinct and the $\mathbf{c}_i$ are all nonzero. If $p = 1$ and we identify $M_1(\mathbb{C})$ with $\mathbb{C}$, then the definitions above reduce themselves to the usual notions of positive and strict positive definiteness of a kernel on Ω frequently used in the literature (see [2] and other references citing it).

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* Corresponding author.

We observe that the quadratic forms in the previous definitions become

$$\sum_{i,j=1}^{n} \sum_{\mu,\nu=1}^{p} \overline{c_i^{\mu}} c_j^{\nu} f_{\mu\nu}(\mathbf{x}_i, \mathbf{x}_j),$$

if we write $F = [f_{\mu\nu}]_{\mu,\nu=1}^{p}$ and $\mathbf{c}_i = (c_i^1, \ldots, c_i^p)$, $i = 1, \ldots, n$.

Positive definite matrix valued kernels appear as an essential component in many problems in a variety of settings (see [6, 7, 12, 15, 18] and references quoting them). The focus in this paper will be on positive definite matrix-valued kernels $F : \Omega \times \Omega \mapsto M_p(\mathbb{C})$ that fit into the following general description:

$$F(x,y) = \sum_{\alpha \in J} A_\alpha f_\alpha(x,y), \quad x, y \in \Omega, \tag{2}$$

where J is a subset of $\mathbb{Z}^q$ for some positive integer q, each A_α is a positive semi-definite matrix that belongs to $M_p(\mathbb{C})$, each $f_\alpha : \Omega \times \Omega \to \mathbb{C}$ is a positive definite kernel and the series is absolutely convergent for all x and y in Ω. The summation symbol needs to be specified in each instance and the set $\{f_\alpha : \alpha \in J\}$ may inherit specific properties defined by the setting. We want to highlight that for the most relevant cases found in the theory and its applications, the set Ω is endowed with a topology while F and the f_α are assumed to be at least continuous.

In this paper, we will provide an abstract criterion for the strict positive definiteness of F as in (2), no matter what Ω, the A_α and the f_α are, and we will discuss some issues related to the criterion in some specific cases fitting in the description above which are described in the examples below. To the best of our knowledge, Examples 3, 4, and 5 have only been investigated in the case $p = 1$.

EXAMPLE 1. $\Omega = S^m$, the unit sphere in $\mathbb{R}^{m+1}$, with F continuous and isotropic. In this case, we have $J = \mathbb{Z}_+$ and

$$f_k(x,y) = P_k^m(\cos d_m(x,y)) = P_k^m(\langle x, y \rangle), \quad x, y \in S^m;\ k \in J,$$

where P_k^m is the Gegenbauer polynomial of degree k associated with the rational number $(m-1)/2$ and d_m is the great circle distance on S^m. The isotropy of F refers to the fact that the variables x and y are tied to each other through the distance d_m. Clearly, $\langle \cdot, \cdot \rangle$ stands for the usual inner product in $\mathbb{R}^{m+1}$. In this setting, the matrices A_k in the expansion of F have real entries. Consequently, since the kernel F is symmetric, one may use real vectors $\mathbf{c}_i$ in the definitions of positive definiteness and strict positive definiteness. This case was quite exploited in [6] and in the references quoted in there.

EXAMPLE 2. $\Omega = H^m$, a compact two-point homogeneous space of dimension m, which we assume being not a sphere, with F continuous and isotropic. In this case, $J = \mathbb{Z}_+$ and

$$f_k(x,y) = P_k^{((m-2)/2, b)}(\cos d_m(x,y)), \quad x, y \in H^m;\ k \in J,$$

where $P_k^{((m-2)/2,b)}$ is a Jacobi polynomial of degree k associated with the pair $((m-2)/2,b)$, b is a number attached to the dimension of H^m, while d_m is the Riemannian distance on H^m so normalized that all geodesics in H^m have the same length π. It is known that H^m can belong to one of the following categories: the real projective spaces $\mathbb{P}^m(\mathbb{R})$, $m=2,3,\ldots$; $b=-1/2$, the complex projective spaces $\mathbb{P}^m(\mathbb{C})$, $m=4,6,\ldots$; $b=0$, the quaternionic projective spaces $\mathbb{P}^m(\mathbb{H})$, $m=8,12,\ldots$; $b=1$, and the Cayley projective plane $\mathbb{P}^m(Cay)$, $m=16$; $b=3$. Here, as in Example 1, the matrices A_k in the expansion of F have real entries. This case was considered in [3] and reassessed later in [10].

EXAMPLE 3. $\Omega=$ a real inner product space $(H,\langle\cdot,\cdot\rangle)$ of dimension at least 2 where F is a continuous ridge function, that is, F is of the form

$$F(x,y)=F'(\langle x,y\rangle),\quad x,y\in H,$$

for some continuous function $F':\mathbb{R}\to M_p(\mathbb{C})$. In this case, we have $J=\mathbb{Z}_+$, real-valued matrices A_k, and

$$f_k(x,y)=\langle x,y\rangle^k,\quad x,y\in H;\ k\in J.$$

The scalar case, that is, the case in which $p=1$, was analyzed in [9, 14]. As far as we know, the other cases were never considered in the literature. We observe that the matrices A_k in the expansion of F in this setting have real entries, and the remarks about the vectors $\mathbf{c}_i$ made in Example 1 apply. This setting allows the consideration of positive definiteness and strict positive definiteness on some subsets of H such as: $H\setminus\{0\}$, subspaces of H, spheres of H, etc. In these cases, the concepts of positive and strict positive definiteness refer to the restrictions of F to the cartesian product of the subset by itself.

EXAMPLE 4. $\Omega=$ a complex inner product space $(H,\langle\cdot,\cdot\rangle)$ of dimension at least 3 where F is again a continuous ridge function. In this case, we have $J=\mathbb{Z}_+^2$ and

$$f_\alpha(x,y)=\langle x,y\rangle^k\overline{\langle x,y\rangle}^l,\quad x,y\in H;\ \alpha=(k,l)\in J.$$

The scalar case $p=1$ was analyzed in [13] but the matrix valued case seems to have been forgotten. As in Example 3, this case allows us to consider the positive definiteness and strict positive definiteness on some relevant subsets of H.

EXAMPLE 5. Here, Ω is the m-dimensional torus

$$T_m:=\{x=(x_1,\ldots,x_m)\in\mathbb{R}^m:-\pi\leqslant x_j<\pi; j=1,2,\ldots,m\},$$

considered as a locally compact topological group, where F is 2π-periodic and continuous on $\mathbb{R}^m$. In this case, we have $J=\mathbb{Z}^m$,

$$f_\alpha(x,y)=e^{i\alpha(x-y)},\quad x,y\in T_m;\ \alpha\in J,$$

and the series (2) needs to be multi-indexed (see [16]). Likewise, the product $\alpha(x-y)$ needs to be understood in the multi-index sense. The strict positive definiteness in the scalar case $p=1$ was taken into consideration in [4] and references quoted in there but the general case is nowhere to be found in the literature.

The reader is advised that there are other settings fitting the description in (2): $\Omega=$ the unit sphere in $\mathbb{C}^m$ with F continuous and isotropic; $\Omega=$ a cartesian product of two spheres with F continuous and isotropic in both variables; etc. Details on these settings will not be included here.

Moving towards the application side, it is known that a positive definite matrix-valued kernel $F:\Omega\times\Omega\to\mathbb{C}$ defines a uniquely defined reproducing kernel Hilbert space $(\mathscr{H},\langle\cdot,\cdot\rangle_F)$ in which $\mathscr{H}$ is a subspace of the vector space of all functions with domain Ω taking values in $\mathbb{C}^p$. Since the strict positive definiteness of F is equivalent to the non-degeneracy of $\mathscr{H}$, strictly positive definite functions F are preferable if the reproducing kernel Hilbert space $\mathscr{H}$ is going to be used as a source of approximations. This explains one possible need for results that characterize the strict positive definiteness of positive definite matrix-valued functions as we will address here.

The paper proceeds as follows. In Section 2, we introduce some notations needed in order to present our abstract characterization for the strict positive definiteness of positive definite kernels as in (2) in Theorem 1. This description is equivalent to simpler conditions in at least two particular cases which we will make explicit at the end of the section. In Section 3, we include an alternative description for the abstract characterization given in Section 2. In Section 4, we discuss further results but we restrict ourselves to some of the concrete settings presented in Section 1.

2. Strict positive definiteness

In this section, we present an abstract necessary and sufficient condition for the strict positive definiteness of a positive definite matrix function F as in (2). The result itself depends upon additional notation which we now introduce.

First of all, the reader should notice that for a function F as in (2) and a vector $\mathbf{c}$ from $\mathbb{C}^p$, the scalar kernel $\mathbf{c}^*F\mathbf{c}$ given by

$$(\mathbf{c}^*F\mathbf{c})(x,y):=\mathbf{c}^*F(x,y)\mathbf{c}=\sum_{\alpha\in J}(\mathbf{c}^*A_\alpha\mathbf{c})\,f_\alpha(x,y),\quad x,y\in\Omega,$$

is positive definite on Ω. Further, if $\mathbf{c}\neq 0$ and F is strictly positive definite, then $\mathbf{c}^*F\mathbf{c}$ is actually strictly positive definite.

Keeping F as in (2), for a vector x_1 of Ω and a nonzero vector $\mathbf{c}_1$ of $\mathbb{C}^p$, we set

$$Q_{x_1}(x_1)=\mathbf{c}_1^*F(x_1,x_1)\mathbf{c}_1.$$

Obviously, $Q_{x_1}(x_1)$ is a nonnegative number that depends upon $\mathbf{c}_1$ whereas our notation does not carry that dependence. Since each A_α is a positive semi-definite matrix and each f_α is a positive definite kernel on Ω, we know already that $\mathbf{c}_1^*A_\alpha\mathbf{c}_1\geqslant 0$ and $f_\alpha(x_1,x_1)\geqslant 0$ for all $\alpha\in J$. Hence, $Q_{x_1}(x_1)>0$ if and only if there exists an index $\alpha\in J$ so that $\mathbf{c}_1^*A_\alpha\mathbf{c}_1>0$ and $f_\alpha(x_1,x_1)>0$.

For $n \geqslant 2$, a subset $\{x_1,\dots,x_n\}$ of Ω and corresponding nonzero vectors $\mathbf{c}_1,\dots,\mathbf{c}_n$ in $\mathbb{C}^p$, we also set

$$Q(x_2,\dots,x_n) = \sum_{\alpha\in J}\sum_{i,j=2}^{n} \mathbf{c}_i^* A_\alpha \mathbf{c}_j f_\alpha(x_i,x_j),$$

and

$$Q_{x_1}(x_2,\dots,x_n) = \sum_{\alpha\in J}\sum_{i=2}^{n} [\mathbf{c}_1^* A_\alpha \mathbf{c}_i f_\alpha(x_1,x_i) + \mathbf{c}_i^* A_\alpha \mathbf{c}_1 f_\alpha(x_i,x_1)].$$

Again, these two definitions depend upon the $\mathbf{c}_i$ whereas the notation does not carry the dependence explicitly. The positive definiteness of F implies that $Q(x_2,\dots,x_n) \geqslant 0$. Further, if F is strictly positive definite and the $\mathbf{c}_i$ are nonzero, then we have actually that $Q(x_2,\dots,x_n) > 0$. Since each A_α is Hermitian and each f_α is positive semidefinite, it is easily seen that

$$Q_{x_1}(x_2,\dots,x_n) = 2\sum_{\alpha\in J}\sum_{i=2}^{n} \mathrm{Re}\,[\mathbf{c}_1^* A_k \mathbf{c}_i f_\alpha(x_1,x_i)].$$

In particular, $Q_{x_1}(x_2,\dots,x_n)$ is a real number.

We are about ready to prove the main result in this section.

THEOREM 1. *If F is as in (2), then following assertions are equivalent:*

- (i) *F is strictly positive definite.*
- (ii) *If $n \in \{1,\dots,|\Omega|\}$, $x_1,\dots,x_n$ are distinct points in Ω and $\mathbf{c}_1,\dots,\mathbf{c}_n$ are nonzero vectors in $\mathbb{C}^p$, then*

$$\begin{cases} Q_{x_1}(x_1) > 0, & \text{if } n = 1 \\ |Q_{x_1}(x_2,\dots,x_n)| < 2Q_{x_1}(x_1)^{1/2} Q(x_2,\dots,x_n)^{1/2}, & \text{if } n \geqslant 2. \end{cases}$$

Proof. Assume F is strictly positive definite and let n, the x_i and the $\mathbf{c}_i$ be as in (ii). If $n = 1$, we may apply the definition of strict positive definiteness using the point x_1 and the nonzero vector $\mathbf{c}_1$ to obtain

$$0 < \mathbf{c}_1^* F(\mathbf{x}_1,\mathbf{x}_1)\mathbf{c}_1 = Q_{x_1}(x_1).$$

If $n > 1$, we apply the definition of strict positive definiteness with the points $x_1,\dots,x_n$ and the nonzero vectors $t\mathbf{c}_1,\mathbf{c}_2,\dots,\mathbf{c}_n$, where t is a nonzero real number. The outcome is

$$0 < Q_{x_1}(x_1)t^2 + Q_{x_1}(x_2,\dots,x_n)t + Q(x_2,\dots,x_n). \tag{3}$$

Since $Q(x_2,\dots,x_n) > 0$, it follows that (3) holds for $t \in \mathbb{R}$. Therefore, we can infer that

$$Q_{x_1}(x_2,\dots,x_n)^2 < 4Q_{x_1}(x_1)Q(x_2,\dots,x_n).$$

This shows that (i) implies (ii).

Conversely, assume (ii) holds and let n be a positive integer at most $|\Omega|$, $x_1,\dots,x_n$ distinct points in Ω and $\mathbf{c}_1,\dots,\mathbf{c}_n$ nonzero vectors in $\mathbb{C}^p$. We need to show that

$$\sum_{\alpha\in J}\sum_{i,j=1}^{n}\mathbf{c}_i^*A_\alpha\mathbf{c}_j f_\alpha(\mathbf{x}_i,\mathbf{x}_j)>0.$$

The case $n=1$ follows from (ii) at once. In the case $n>1$, observe that

$$\sum_{\alpha\in J}\sum_{i,j=1}^{n}\mathbf{c}_i^*A_\alpha\mathbf{c}_j f_\alpha(x_i,x_j)=Q_{x_1}(x_1)+Q_{x_1}(x_2,\dots,x_n)+Q(x_2,\dots,x_n)=p(1),$$

in which

$$p(t)=Q_{x_1}(x_1)t^2+Q_{x_1}(x_2,\dots,x_n)t+Q(x_2,\dots,x_n).$$

By (ii), we know that

$$Q_{x_1}(x_2,\dots,x_n)^2-4Q_{x_1}(x_1)Q(x_2,\dots,x_n)<0.$$

Since $Q_{x_1}(x_1)>0$, it follows that $p(t)>0$ for all $t\in\mathbb{R}$. In particular, $p(1)>0$. Thus (ii) implies (i). $\square$

The equivalence for strict positive definiteness provided by Theorem 1 is abstract in the sense that Assertion (ii) cannot be easily assessed in applications. It would be more desirable to have an equivalence easier to be checked. For instance, this is what occurs in most of the cases described in Example 1 and also in all the cases in Example 2. We make that clear through formal statements.

THEOREM 2. *Let F be as in (2) but under the setting of Example 1. If $m\geqslant 2$, Assertions (i) and (ii) in Theorem 1 are equivalent to the following additional assertions:*

(iii) *If $\mathbf{c}$ is a nonzero vector of $\mathbb{C}^p$, then $\{k\in\mathbb{Z}_+ : \mathbf{c}^*A_k\mathbf{c}>0\}$ contains infinitely many even and infinitely many odd integers.*

(iv) *If $\mathbf{c}$ is a nonzero vector of $\mathbb{C}^p$, then $\mathbf{c}^*F\mathbf{c}$ is a strictly positive definite scalar kernel.*

Proof. This is a consequence of Theorem 3 in [6]. $\square$

THEOREM 3. *Let F be as in (2) but under the setting of Example 2. Assertions (i) and (ii) in Theorem 1 are equivalent to the following additional assertions:*

(iii) *If $\mathbf{c}$ is a nonzero vector of $\mathbb{C}^p$, then $\{k\in\mathbb{Z}_+ : \mathbf{c}^*A_k\mathbf{c}>0\}$ contains infinitely many integers.*

(iv) *If $\mathbf{c}$ is a nonzero vector of $\mathbb{C}^p$, then $\mathbf{c}^*F\mathbf{c}$ is a strictly positive definite scalar kernel.*

Proof. This follows from Theorem 4.4 in [3] and Theorem 3 in [1]. □

The reader should not expect equivalences for strict positive definiteness as simpler as the ones in Theorems 2 and 3 for the other settings described in Section 1. Indeed, the proofs of these two theorems take into account the metric structure of the spaces involved and specific asymptotic properties of the functions f_α. For instance, Example 6 below points that simpler equivalences for strict positive definiteness in the setting of Example 3 are not possible, even if one considers strict positive definiteness on subsets of H.

EXAMPLE 6. Let Ω and F be as in Example 3. If $\mathbf{c}$ is a nonzero vector in $\mathbb{C}^p$, then $\mathbf{c}^*F\mathbf{c}$ belongs to the same setting, but with $p=1$. If F is strictly positive definite, the same is true of $\mathbf{c}^*F\mathbf{c}$. Reporting to the main theorem in [14], we can infer that $\{k \in \mathbb{Z}_+ : \mathbf{c}^*A_k\mathbf{c} > 0\}$ contains infinitely many even and infinitely many odd integers. However, this condition being true for every nonzero vector $\mathbf{c}$ of $\mathbb{C}^p$ is far from being equivalent to the strict positive definiteness of F. Indeed, define

$$A_k = \frac{1}{k!}\begin{pmatrix} 2^{2k} & -2^k \\ -2^k & 1 \end{pmatrix}, \quad k \in \mathbb{Z}_+.$$

Obviously each A_k is positive semi-definite and the series $F'(t) = \sum_k A_k t^k$ converges for all $t \in \mathbb{R}$. If we write $\mathbf{c}_1 = (1,0)$ and $\mathbf{c}_2 = (0,1)$, it is easily seen that

$$\mathbf{c}_2^\intercal A_k \mathbf{c}_2 = 2^{-2k}\mathbf{c}_1^\intercal A_k \mathbf{c}_1 = \frac{1}{k!}, \quad k \in \mathbb{Z}_+,$$

and

$$\mathbf{c}_1^\intercal A_k \mathbf{c}_2 = \mathbf{c}_2^\intercal A_k \mathbf{c}_1 = -\frac{2^k}{k!}, \quad k \in \mathbb{Z}_+.$$

In particular, if H is a real inner product space and we choose $\{x_1, x_2\} \subset H$, with x_1 unitary and $x_2 = tx_1$, where $t \in \mathbb{R}$, it follows that

$$g(t) = \sum_{i,j=1}^{2}\sum_{k=0}^{\infty} \mathbf{c}_i^\intercal A_k \mathbf{c}_j \left\langle x_i, x_j \right\rangle^k = \sum_{k=0}^{\infty}\left(2^{2k} - 2^k t^k - 2^k t^k + t^k t^k\right)\frac{1}{k!} \geqslant 0$$

for all $t \in \mathbb{R}$. Since, $g(2) = 0$, we can conclude that the matrix-valued positive definite kernel

$$F(x,y) = F'(\langle x,y\rangle) = \sum_{k=0}^{\infty} A_k \langle x,y\rangle^k, \quad x,y \in [\{x_1\}] \setminus \{0\},$$

is not strictly positive definite. On the other hand, if $\mathbf{c} = (a,b) \in \mathbb{R}^2 \setminus \{(0,0)\}$, then

$$\mathbf{c}^\intercal A_k \mathbf{c} = \frac{(a2^k - b)^2}{k!}, \quad k \in \mathbb{Z}_+.$$

If $a = 0$, then $\mathbf{c}^\intercal A_k \mathbf{c} = b^2/k! > 0$ for all k. The same holds true if $b = 0$. Otherwise, there exists at most one integer k for which $\mathbf{c}^\intercal A_k \mathbf{c} = 0$. In particular, $\{k : \mathbf{c}^\intercal A_k \mathbf{c} > 0\}$ contains infinitely many even and infinitely many odd integers whenever $\mathbf{c} \neq 0$.

3. Strict positive definiteness: part 2

In this section, we present a counterpositive version of Theorem 1 in which the motivation comes from Example 6.

Let us assume for a moment that a kernel F as in (2) is not strictly positive definite on Ω and that the strict positive definiteness fails for two distinct points x_1, x_2 of Ω and nonzero vectors $\mathbf{c}_1, \mathbf{c}_2$ of $\mathbb{C}^p$, that is,

$$\sum_{i,j=1}^{2} \sum_{\alpha \in J} \mathbf{c}_i^* A_\alpha \mathbf{c}_j f_\alpha(x_i, x_j) = 0.$$

If we set $\mathbf{d}_1 = t\mathbf{c}_1$ with $t \in \mathbb{R}$ and $\mathbf{d}_2 = \mathbf{c}_2$, then the polynomial

$$h(t) := \sum_{i,j=1}^{2} \sum_{\alpha \in J} \mathbf{d}_i^* A_\alpha \mathbf{d}_j f_\alpha(x_i, x_j)$$

is nonnegative-valued by the positive definiteness of F on Ω. Now notice that h can be written in the form

$$h(t) = t^2 \sum_{\alpha \in J} \mathbf{c}_1^* A_\alpha \mathbf{c}_1 f_\alpha(x_1, x_1) + 2t \sum_{\alpha \in J} \mathrm{Re}\, [\mathbf{c}_1^* A_\alpha \mathbf{c}_2 f_\alpha(x_1, x_2)] + \sum_{\alpha \in J} \mathbf{c}_2^* A_\alpha \mathbf{c}_2 f_\alpha(x_2, x_2).$$

Its minimum value is attained at $t = 1$, that is, $h(1) = h'(1) = 0$. In particular, h is actually of the form

$$h(t) = (t-1)^2 \sum_{\alpha \in J} \mathbf{c}_1^* A_\alpha \mathbf{c}_1 f_\alpha(x_1, x_1).$$

Therefore, we can infer that

$$\sum_{\alpha \in J} \mathbf{c}_1^* A_\alpha \mathbf{c}_1 f_\alpha(x_1, x_1) = \sum_{\alpha \in J} \mathbf{c}_2^* A_\alpha \mathbf{c}_2 f_\alpha(x_2, x_2), \tag{4}$$

and

$$\sum_{\alpha \in J} \mathrm{Re}\, [\mathbf{c}_1^* A_\alpha \mathbf{c}_2 f_\alpha(x_1, x_2)] = -\sum_{\alpha \in J} \mathbf{c}_1^* A_\alpha \mathbf{c}_1 f_\alpha(x_1, x_1). \tag{5}$$

In short, the arguments above suggest that if a function F as in (2) is not strictly positive definite on Ω, then either (4) and (5) must hold for two distinct points x_1 and x_2 of Ω and two nonzero vectors $\mathbf{c}_1$ and $\mathbf{c}_2$ of $\mathbb{C}^p$ or some sort of extension of (4) and (5) must hold for some $n \geqslant 3$, distinct points $x_1, \ldots, x_n$ of Ω and nonzero vectors $\mathbf{c}_1, \ldots, \mathbf{c}_n$ of $\mathbb{C}^p$. The extension itself will appear explicitly in Theorem 4 below.

THEOREM 4. *If F is as in (2), then following assertions are equivalent:*

(i) *F is not strictly positive definite.*

(ii) *There exist $n \in \{1, \ldots, |\Omega|\}$, distinct points $x_1, \ldots, x_n$ in Ω and nonzero vectors $\mathbf{c}_1, \ldots, \mathbf{c}_n$ in $\mathbb{C}^p$ such that*

$$\begin{cases} Q_{x_1}(x_1) = 0, & \text{if } n = 1 \\ \\ Q_{x_1}(x_2, \ldots, x_n) = -2Q_{x_1}(x_1) = -2Q(x_2, \ldots, x_n) & \text{if } n \geqslant 2. \end{cases}$$

Proof. Assume F is not strictly positive definite on Ω. According to the definition of strict positive definiteness, we can find $n \in \{1,\ldots,|\Omega|\}$, distinct points $x_1,\ldots,x_n$ in Ω and nonzero vectors $\mathbf{c}_1,\ldots,\mathbf{c}_n$ in $\mathbb{C}^p$ such that

$$\sum_{\alpha\in J}\sum_{i,j=1}^{n} \mathbf{c}_i^* A_\alpha \mathbf{c}_j f_\alpha(\mathbf{x}_i,\mathbf{x}_j) = Q_{x_1}(x_1) + Q_{x_1}(x_2,\ldots,x_n) + Q(x_2,\ldots,x_n) = 0.$$

If $n=1$, this corresponds to $Q_{x_1}(x_1)=0$. Otherwise, we set

$$g(s,t) = Q_{x_1}(x_1)t^2 + Q_{x_1}(x_2,\ldots,x_n)st + Q(x_2,\ldots,x_n)s^2. \tag{6}$$

This polynomial is obtained by replacing $\mathbf{c}_1$ with $ts^{-1}\mathbf{c}_1$ in the double sum above, where $t,s\in\mathbb{R}$ and $s\neq 0$, and multiplying the resulting double sum by s^2. The polynomial g is nonnegative-valued by the positive definiteness of F. Direct inspection reveals that $g(1,1)=0$. Hence, we must have

$$\frac{\partial g}{\partial t}(1,1) = \frac{\partial g}{\partial s}(1,1) = 0,$$

that is,

$$2Q_{x_1}(x_1) + Q_{x_1}(x_2,\ldots,x_n) = 0 = 2Q(x_2,\ldots,x_n) + Q_{x_1}(x_2,\ldots,x_n),$$

and (ii) holds. Conversely, assume (ii) holds. We may assume that $n \geqslant 2$, once F is obviously not strictly positive definite otherwise. If $x_1,\ldots,x_n$ are distinct points in Ω and $\mathbf{c}_1,\ldots,\mathbf{c}_n$ are nonzero vectors in $\mathbb{C}^p$ satisfying

$$Q_{x_1}(x_2,\ldots,x_n) = -2Q_{x_1}(x_1) = -2Q(x_2,\ldots,x_n),$$

then

$$\sum_{\alpha\in J}\sum_{i,j=1}^{n} \mathbf{c}_i^* A_\alpha \mathbf{c}_j f_\alpha(\mathbf{x}_i,\mathbf{x}_j) = Q_{x_1}(x_1) + Q_{x_1}(x_2,\ldots,x_n) + Q(x_2,\ldots,x_n) = 0.$$

Therefore, F is not strictly positive on Ω. □

An obvious consequence is as follows.

COROLLARY 1. *Let F be as in (2). Assume $Q_{x_1}(x_1)>0$ whenever $x_1\in\Omega$ and $\mathbf{c}_1$ is a nonzero vector of $\mathbb{C}^p$. If $Q_{x_1}(x_2,\ldots,x_n)\geqslant 0$ whenever $n\in\{2,\ldots,|\Omega|\}$, $x_1,\ldots,x_n$ are distinct points of Ω, and $\mathbf{c}_1,\ldots,\mathbf{c}_n$ are nonzero vectors of $\mathbb{C}^p$, then F is strictly positive definite.*

Proof. If F is not strictly positive on Ω and $Q_{x_1}(x_1)>0$ whenever $x_1\in\Omega$ and $\mathbf{c}_1$ is a nonzero vector of $\mathbb{C}^p$, Theorem 4 asserts the existence of $n\in\{2,\ldots,|\Omega|\}$, distinct points $x_1,\ldots,x_n$ in Ω and nonzero vectors $\mathbf{c}_1,\ldots,\mathbf{c}_n$ in $\mathbb{C}^p$ such that

$$Q_{x_1}(x_2,\ldots,x_n) = -2Q_{x_1}(x_1) < 0.$$

The result follows. □

4. Further results

In this section, we discuss some additional features related to the characterizations we have presented in Sections 2 and 3. Hopefully, this will foment additional research on the topic and will lead to simpler characterizations for strict positive definiteness of kernels as in (2) in all the settings mentioned in Section 1. In any case, the reader is advised that a universal simplification of the equivalences given in either Theorem 1 or 4 is very unlikely to happen. Indeed, the examples analyzed in this paper suggests that a simplification would depend upon Ω and on additional properties in the function F implied by the setting. Thus, it would depend on the special features of the f_α as well.

Let us begin with a piece of information that, in a certain sense, makes the strict positive definiteness in the cases $p=1$ and $p>1$ quite distinct from each other. If $p=1$, it is very easy to see that the strict positive definiteness of F as in (2) depends upon the set $\{\alpha : A_\alpha > 0\}$, and not on the actual value that each real number A_α assumes. This is one of the reasons why the strict positive definiteness in the case $p=1$ has been already described by elementary means in all the settings we have mentioned in Section 1.

If a setting allows a simple characterization for strict positive definiteness in the case $p=1$ or at least the determination of a necessary condition for that, then a necessary condition for the strict positive definiteness in the case $p>1$ can be inferred at once, as we have done in at at least two cases in Section 2. Indeed, if the strict positive definiteness of F as in (2) in the case $p=1$ is defined by a property P that the set $\{\alpha : A_\alpha > 0\}$ has, then a necessary condition for the strict positive definiteness of F as in (2) in the case $p>1$ is precisely this one: $\{\alpha : \mathbf{c}^* A_\alpha \mathbf{c} > 0\}$ has the property P whenever $\mathbf{c}$ is a nonzero vector of $\mathbb{C}^p$.

Below, we will address what this remark implies in each one of the three remaining examples from Section 1. Needless to say that F is assumed to be positive definite according to each setting.

Example 3: A necessary condition for the strict positive definiteness of F on H in the case $p>1$ is that $\{k \in \mathbb{Z}_+ : \mathbf{c}^* A_k \mathbf{c} > 0\}$ contains the index 0 along with infinitely many even and infinitely many odd integers, whenever $\mathbf{c}$ is a nonzero vector in $\mathbb{C}^p$, a fact that follows from the main result in [14]. As for the case of strict positive definiteness on $H \setminus \{0\}$, the necessary condition is the same except that the integer 0 may be excluded from $\{k \in \mathbb{Z}_+ : \mathbf{c}^* A_k \mathbf{c} > 0\}$. If X is a subset of H for which $\{x \in X : -x \in X\}$ is infinite, the necessary condition for the strict positive definiteness of F on X is the same, and again one needs to consider two cases depending whether 0 belongs to X. This fact is implied by Theorem 1 and Proposition 2 in [9]. It includes the case in which X is a subspace isometrically isomorphic to $\mathbb{R}$. Just for the record, the necessary condition mentioned here is equivalent to the following property: $\{k \in \mathbb{Z}_+ : \mathbf{c}^* A_k \mathbf{c} > 0\}$ contains the index 0 and for every $m \in \mathbb{Z}_+$, both matrices $\sum_{2k \geqslant m} A_{2k}$ and $\sum_{2k+1 \geqslant m} A_{2k+1}$ are positive definite. Another interesting property that deserves to be mentioned in this case is this one: if F is strictly positive definite on X and $0 \in X$, then A_0 is positive definite.

We also can add the following additional result in this setting.

THEOREM 5. *If H is separable, X is a sphere in H centered at 0, and F is positive definite on H, then the following assertions are equivalent:*

(i) *F is strictly positive definite on X.*

(ii) *If $\mathbf{c} \in \mathbb{C}^p$, then $\{k \in \mathbb{Z}_+ : \mathbf{c}^* A_k \mathbf{c} > 0\}$ contains infinitely many even and infinitely many odd integers.*

Proof. If H_1 and H_2 are real inner product spaces which are isometrically isomorphic, then a function F as in (2) is strictly positive definite on H_1 if and only if it is so on H_2. If $\phi : H_1 \to H_2$ is the isometric isomorphism and X is a nonempty subset of H_1, then f is strictly positive definite on X if and only if it is so on $\phi(X)$. In view of this, it suffices to prove the theorem in the cases in which $H = \mathbb{R}^m$, $2 \leqslant m < \infty$, and $H =$the real ℓ_2. Let S_R be the sphere of radius $R > 0$ and centered at 0 in each one of these spaces. If F is as in (2), then

$$F(\langle x,y \rangle) = \sum_{k=0}^{\infty} R^{2k} A_k \left\langle R^{-1}x, R^{-1}y \right\rangle^k, \quad x,y \in S_R.$$

On the other hand, if $\mathbf{c}$ is a nonzero vector in $\mathbb{C}^p$, then

$$\{k : R^{2k}\mathbf{c}^* A_k \mathbf{c} > 0\} \cap 2\mathbb{Z}_+ = \{k : \mathbf{c}^* A_k \mathbf{c} > 0\} \cap 2\mathbb{Z}_+$$

and

$$\{k : R^{2k}\mathbf{c}^* A_k \mathbf{c} > 0\} \cap (2\mathbb{Z}_+ + 1) = \{k : \mathbf{c}^* A_k \mathbf{c} > 0\} \cap (2\mathbb{Z}_+ + 1).$$

Therefore, it suffices to show the result holds in the case in which X is the unit sphere in either case. Since $\{x \in X : -x \in X\}$ is infinite in both cases, it suffices to show that (ii) implies (i). The first step is to write

$$F(\langle x,y \rangle) = F(\cos d(x,y)) = \sum_{k=0}^{\infty} A_k \cos^k(d(x,y)), \quad x,y \in S^m, \tag{7}$$

where d stands for the geodesic distance on the sphere in either case. Now, Theorem 5 in [6] takes care of the case in which X is the unit sphere in ℓ_2. As for the other, we invoke the well-known formula

$$(\cos\theta)^k = b^m_{k,k} P_k(\cos\theta) + b^m_{k,k-2} P^m_{k-2}(\cos\theta) + \cdots, \quad \theta \in [0,\pi], \tag{8}$$

in which all the $b^m_{k,j}$, $j = k, k-2, \ldots$, are positive and P^m_k denotes the Gegenbauer polynomial of degree k associated with the rational number $(m-2)/2$ (see [17]). Returning to (7), we obtain

$$F(\langle x,y \rangle) = \sum_{k=0}^{\infty} B_k P^m_k(\cos d_m(x,y)),$$

where

$$B_k = b^m_{k,k} A_k + b^m_{k+2,k} A_{k+2} + \cdots = \sum_{j=0}^{\infty} b^m_{k+2j,k} A_{k+2j}, \quad k \in \mathbb{Z}_+.$$

Each B_k is obviously positive semi-definite. On the other hand, if $\mathbf{c}^* A_{k+2j_0}\mathbf{c} > 0$ for some $\mathbf{c} \in \mathbb{R}^p \setminus \{0\}$, and k and $j_0 \in \mathbb{Z}_+$, then $\mathbf{c}^* B_k \mathbf{c} > 0$. In particular, if $\{k : \mathbf{c}^* A_k \mathbf{c} > 0\} \cap 2\mathbb{Z}_+$ (respectively, $\{k : \mathbf{c}^* A_k \mathbf{c} > 0\} \cap (2\mathbb{Z}_+ + 1)$) is infinite, then the same is true of $\{k : \mathbf{c}^* B_k \mathbf{c} > 0\} \cap 2\mathbb{Z}_+$ (respectively, $\{k : \mathbf{c}^* B_k \mathbf{c} > 0\} \cap 2\mathbb{Z}_+ + 1$). Therefore, if (ii) holds, then Theorem 3 in [6] shows that F is strictly positive definite on X. □

Example 4: A necessary condition for the strict positive definiteness of F on H in the case $p > 1$ is that $\{k - l : \mathbf{c}^* A_{(k,l)}\mathbf{c} > 0\}$ intersects every full arithmetic progression in $\mathbb{Z}$, whenever $\mathbf{c}$ is a nonzero vector in $\mathbb{C}^p$. This follows from the main result proved in [14].

Example 5: A necessary condition for the strict positive definiteness of F on T_m in the case $p > 1$ is that $\{\alpha \in \mathbb{Z}^m : \mathbf{c}^* A_\alpha \mathbf{c} > 0\}$ intersects all the translations of each subgroup of $\mathbb{Z}^m$ that has the form $(n_1\mathbb{Z}, \ldots, n_m\mathbb{Z})$, with $n_1, \ldots, n_m \in \mathbb{Z}_+$, whenever $\mathbf{c}$ is a nonzero vector in $\mathbb{C}^p$. This is implied by Theorem 1 in [4].

5. Conclusion and final comments

In this paper we have provided an abstract criterion for the strict positive definiteness of matrix functions that define matrix-valued positive definite kernels given by certain absolutely convergent series expansions on a set. Some contexts previously discussed in the literature belong to the setting in which the criterion holds. A self-contained characterization for strict positive definiteness already exists in some of them but does not in others. The criterion is very difficult to be used in practice, once it depends upon the setting itself and it is not explicit with respect to what properties in the expansion of the kernel one should look for. For that reason, we have exploited quite a bit some of the contexts exposed in the paper in an attempt to show to the readers why self-contained characterizations were possible in some settings but were not in others. Hopefully, future research will lead to additional characterizations of the strict positive definiteness of matrix-valued positive definite kernels in the remaining settings mentioned here and in others which are relevant in applications.

We close the paper with a re-interpretation for positive definiteness in the setting of Example 4. First of all, one should notice that, keeping the notation in Theorem 1, the positive definiteness of F corresponds to

$$\begin{cases} Q_{x_1}(x_1) \geqslant 0, & \text{if } n = 1 \\ \\ |Q_{x_1}(x_2, \ldots, x_n)| \leqslant 2Q_{x_1}(x_1)^{1/2} Q(x_2, \ldots, x_n)^{1/2}, & \text{if } n \geqslant 2. \end{cases}$$

whenever $n \in \{1, \ldots, |\Omega|\}$, $x_1, \ldots, x_n$ are points in Ω and $\mathbf{c}_1, \ldots, \mathbf{c}_n$ are vectors in $\mathbb{C}^p$. That being said, if we restrict ourselves to the setting of Example 4 and take $n = 2$ and

$$F(x,y) = I_p \langle x,y\rangle^k \overline{\langle x,y\rangle^k} = I_p |\langle x,y\rangle|^{2k}, \quad x,y \in H,$$

where I_p is the identity matrix of $M_p(\mathbb{C})$ and $(k,k) \in \mathbb{Z}_+^2$, then we obtain

$$\left[2\mathrm{Re}\left(\mathbf{c}_1^* I_p \mathbf{c}_2 |\langle x_1, x_2\rangle|^{2k}\right)\right]^2 \leqslant 4\left(\mathbf{c}_1^* I_p \mathbf{c}_1 |\langle x_1, x_1\rangle|^{2k}\right)\left(\mathbf{c}_2^* I_p \mathbf{c}_2 |\langle x_2, x_2\rangle|^{2k}\right).$$

If we take $p = 1$ and $\mathbf{c}_1 = \mathbf{c}_2 = 1$, the above inequality becomes the Cauchy-Schwarz inequality

$$|\langle x_1, x_2\rangle|^{4k} \leqslant \langle x_1, x_1\rangle^{2k}\langle x_2, x_2\rangle^{2k}.$$

Expanding to a general n, p, and $\mathbf{c}_1, \ldots, \mathbf{c}_n \in \mathbb{C}^p$, it is now seen that

$$\left(\operatorname{Re}\sum_{i=2}^{n} \mathbf{c}_1^* I_p \mathbf{c}_i |\langle x_1, x_i\rangle|^{2k}\right)^2 \leqslant \left(\mathbf{c}_1^* I_p \mathbf{c}_1 \langle x_1, x_1\rangle^{2k}\right)\left(\sum_{i,j=2}^{n} \mathbf{c}_i^* I_p \mathbf{c}_j |\langle x_i, x_j\rangle|^{2k}\right).$$

The latter can be labeled as an extended Cauchy-Schwarz inequality.

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W. Franca
Departamento de Matemática – ICE
Universidade Federal de Juiz de Fora
36036-330 Juiz de Fora MG, Brazil
e-mail: wvfranca@gmail.com

V. A. Menegatto
Departamento de Matemática – ICE
Universidade Federal de Juiz de Fora
36036-330 Juiz de Fora MG, Brazil
e-mail: menegatt@gmail.com