Methods and Applications of Analysis.
Vol. 29, No. 2, pp. 179–194, June 2022

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AN EXTENSION OF AITKEN'S INTEGRAL FOR GAUSSIANS AND POSITIVE DEFINITENESS*

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Abstract. We recast an extension of Aitken's integral frequently used in quantum field theory and use it to deduce general criteria for constructing positive definite and strictly positive definite kernels on a set X making use of completely monotone functions and special multivariate conditionally negative definite kernels on X. The criteria extend to positive definite kernels on a cartesian product of sets. In particular, we obtain an extension of a classical model of T. Gneiting for the construction of space-time covariance functions. New and old models are obtained as applications of the main results in the paper.

Key words. Positive definite, conditionally negative definite, Hadamard exponential, Schur product Theorem, Oppenheim's inequality, Gneiting's model.

Mathematics Subject Classification. 26A48, 42A82, 62J10.

1. Introduction. Many explicit constructions of positive definite kernels on a nonempty set X found in the literature are based on a prescribed completely monotone function and a nonnegative valued conditionally negative definite kernel on X. For instance, if μ is a probability measure on $[0,\infty)$ such that $0 < \int_{[0,\infty)} s d\mu(s) < \infty$, then a result proved in [3, p.75] shows that for a given conditionally negative definite kernel $g : X \times X \to [0,\infty)$, all the kernels

$$(x,x') \in X \times X \mapsto \int_{[0,\infty)} e^{-s\, r g(x,x')} d\mu(s), \quad r > 0,$$

are positive definite. We observe that the formula above expresses the composition of the conditionally negative definite kernel $(x,x') \in X \times X \mapsto rg(x,x')$, $r > 0$, with the completely monotone function

$$t \in (0,\infty) \mapsto \int_{[0,\infty)} e^{-s\,t} d\mu(s).$$

Convenient choices for the measure μ lead to some very important positive definite kernels. Indeed, by choosing μ as the Dirac measure centered at 1, we see that if $g : X \times X \to [0,\infty)$ is conditionally negative definite, then all the kernels

$$(x,x') \in X \times X \mapsto e^{-rg(x,x')}, \quad r > 0,$$

are positive definite. The choice $d\mu(s) = e^{-s} ds$ and the very same assumption on g, lead to the positive definiteness of the kernels

$$(x,x') \in X \times X \mapsto \frac{1}{r + g(x,x')}, \quad r > 0.$$

It is worth mentioning that, under the setting above, the strict positive definiteness of the positive definite kernels is usually not analyzed. In applications, results of this

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type usually appear adapted to the case where X is endowed with a metric. This aspect is exploited in [13, 27] and other references within.

As for positive definiteness on a cartesian product, the so called Gneiting's criterion is the most popular one that keeps the same approach. For a bounded completely monotone function $\phi : (0, \infty) \to \mathbb{R}$ and a positive valued function f with a completely monotone derivative, Gneiting's model asserts that the formula

$$G_r((x,y),(x',y')) = \frac{1}{f(\|y-y'\|^2)^r}\phi\left(\frac{\|x-x'\|^2}{f(\|y-y'\|^2)}\right), \quad x,x' \in \mathbb{R}^q;\ y,y' \in \mathbb{R}^d \quad (1.1)$$

defines a positive definite kernel on $\mathbb{R}^q \times \mathbb{R}^d$, whenever $r \geq d/2$ and $\|\cdot\|$ denotes the usual norms in both $\mathbb{R}^q$ and $\mathbb{R}^d$ ([8]). The boundedness of ϕ is required in order to make $\phi(0^+) < \infty$. Needless to say that a well-known result of Micchelli ([14]) asserts that if $-\phi$ is completely monotone, then the kernel $(y,y') \in \mathbb{R}^d \times \mathbb{R}^d \mapsto \phi(\|y-y'\|^2)$ is conditionally negative definite on $\mathbb{R}^d$. The references [1, 5, 20, 19, 21, 28] include extensions and generalizations of Gneiting's result along with additional references that justify its importance, while [18] is a survey on the topic. Completely monotone functions are stressed in [15, 26].

In this paper, we present abstract criteria for constructing positive definite and strictly positive definite functions on an arbitrary set from a prescribed completely monotone function and a multivariate conditionally negative definite function on the set employing an extension of Aitken's integral for Gaussians. Thus, the results to be presented in this paper can be interpreted as extensions and generalizations of the motivational results described above.

Section 2 contains the basic definitions used in the paper and some technical results involving the extended Aitken's integral. In Section 3, we state and prove the main results in the paper concerning positive definiteness and strict positive definiteness on a single nonempty set X. Examples are discussed in Section 4, some of them new, some of them resembling models previously studied in specific settings. Section 5 extends some of the results proved in Section 3 to positive definiteness on a product of sets. A generalized version of the classical result of Gneiting for constructing space-time covariances is obtained.

2. Definitions and Aitken's integral. Throughout the paper, X and Y will denote arbitrary sets containing at least two points while $M_q(\mathbb{C})$ will denote the set of all $q \times q$ matrices with complex entries. If the entries are all real, we will prefer to write $M_q(\mathbb{R})$ instead. A kernel $K : X \times X \to M_q(\mathbb{C})$ is *positive definite* if for every positive integer n at most the cardinality of X and distinct points $x_1, \ldots, x_n$ in X, the block matrix $[K(x_\mu, x_\nu)]_{\mu,\nu=1}^n$ of order nq is positive semi-definite, that is,

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

whenever $c_1, \ldots, c_n$ are vectors in $\mathbb{C}^q$. Here, the star notation refers to conjugate transposition of column vectors in $\mathbb{C}^q$. The positive definite kernel K is *strictly positive definite* if the inequalities above are strict whenever at least one of the vectors c_μ is nonzero. Similarly, the kernel K is *conditionally negative definite* if it is Hermitian and the quadratic forms above are nonpositive whenever the vectors c_μ satisfy $\sum_{\mu=1}^n c_\mu = 0$. The conditionally negative definite kernel K is *strictly conditionally negative definite* if the quadratic forms are negative whenever $n \geq 2$ and at least one

c_μ is nonzero. The classes of kernels introduced above will be denoted by $PD_q(X)$, $SPD_q(X)$, $CND_q(X)$, and $SCND_q(X)$, respectively. The standard notions of positive definiteness and conditional negative definiteness are recovered when one takes $q = 1$ and identifies $M_q(\mathbb{C})$ with $\mathbb{C}$ in the previous definitions.

A few remarks deserve to be mentioned at once. A necessary condition in order that a kernel K belongs to $CND_1(X)$ is that

$$K(x,x) + K(x',x') - \operatorname{Re} K(x,x') \leq 0, \quad x, x' \in X.$$

On the other hand, a necessary condition in order that K belongs to $SCND_1(X)$ is that the inequality above be strict when $x \neq x'$.

Another useful information is given by the elementary lemma below. Details will be left to the readers.

Lemma 2.1. *For a matrix function $G : X \times X \to M_q(\mathbb{C})$ and a vector u from $\mathbb{C}^q$, the following assertions hold:*

(i) *If G belongs to $CND_q(X)$, then $(x,x') \in X \times X \mapsto u^*G(x,x')u$ lies in $CND_1(X)$.*

(ii) *If G belongs to $SCND_q(X)$ and u is nonzero, then $(x,x') \in X \times X \mapsto u^*G(x,x')u$ belongs to $SCND_1(X)$.*

We refer the reader to [2, 3] for additional information on kernels belonging to $PD_1(X)$ and $CND_1(X)$. Results on the classes $CND_q(X)$ and $SCND_q(X)$ are scattered in the literature. Reference [10] is a recent work on the topic.

Next, we move to an extension of the well-known formula from Fourier analysis that links positive definite kernels and isometric embeddings, namely,

$$\int_{\mathbb{R}^q} e^{-r\|v\|^2 + i\, v^\intercal w} dv = \left(\frac{\pi}{r}\right)^{q/2} e^{-w^\intercal (4r)^{-1} w}, \quad r > 0;\ w \in \mathbb{R}^q, \tag{2.2}$$

where $v^\intercal$ denotes the transposition of v. Even though the left hand side of (2.2) has a complex integrand, its right hand side is real. We will use the following matrix version of (2.2), an extension of the so-called Aitken's integral for computing Gaussian integrals ([24, p.340]).

Lemma 2.2. *Let A be a matrix in $M_q(\mathbb{R})$ and b a vector in $\mathbb{R}^q$. If A is positive definite, then*

$$\int_{\mathbb{R}^q} e^{-u^\intercal A u + i\, b^\intercal u} du = \frac{\pi^{q/2}}{(\det\, A)^{1/2}} e^{-b^\intercal (4A)^{-1} b}.$$

Proof. If A is positive definite, we can decompose it in the form $A = P^\intercal BB\, P$, where P is an orthogonal matrix in $M_q(\mathbb{R})$ and BB is a diagonal matrix with main diagonal containing the eigenvalues of A counting multiplicities. Performing the change of variables $v = BPu$, $u \in \mathbb{R}^q$, we obtain

$$-u^\intercal A u + i\, b^\intercal u = -(BPu)^\intercal (BPu) + i\,(B^{-1}Pb)^\intercal v = -v^\intercal v + i\,(B^{-1}Pb)^\intercal v, \quad u \in \mathbb{R}^q.$$

Introducing this formula in the integral in the statement of the lemma and recalling (2.2), we are reduced to

$$\begin{aligned}\int_{\mathbb{R}^q} e^{-u^\intercal A u + i\, b^\intercal u} du &= \frac{1}{\det(BP)} \int_{\mathbb{R}^q} e^{-v^\intercal v + i\,(B^{-1}Pb)^\intercal v} dv \\ &= \frac{\pi^{q/2}}{\det(BP)} e^{-(B^{-1}Pb)^\intercal B^{-1}Pb/4}, \quad b \in \mathbb{R}^q.\end{aligned}$$

The proof is finished after we ratify the elementary identities $[\det(BP)]^2 = \det A$ and $(B^{-1}Pb)^{\intercal}B^{-1}Pb = b^{\intercal}A^{-1}b$. □

We close the section with an independent lemma that provides information on the positive (semi-)definiteness of the Hadamard exponential of matrices of negative type (see [22]). Recall that a real symmetric matrix $[A_{\mu\nu}]_{\mu,\nu=1}^{n}$ of order n is of *negative type* (almost negative definite) if

$$\sum_{\mu,\nu=1}^{n} c_\mu A_{\mu\nu} c_\nu \leq 0,$$

for all real numbers satisfying $\sum_{\mu=1}^{n} c_\mu = 0$. It is of *strict negative type* if the previous inequalities are strict when the real numbers c_μ satisfy $\sum_{\mu=1}^{n} c_\mu = 0 < \sum_{\mu=1}^{n} |c_\mu|$.

LEMMA 2.3. *Let $A = [A_{\mu\nu}]_{\mu,\nu=1}^{n}$ be a matrix of negative type. The following assertions hold for the Hadamard exponential $B = [e^{-A_{\mu\nu}}]_{\mu,\nu=1}^{n}$:*
(*i*) *B is positive semi-definite.*
(*ii*) *B is positive definite if and only if $A_{\mu\mu} + A_{\nu\nu} < 2A_{\mu\nu}$, for $\mu \neq \nu$.*
(*iii*) *If A is of strict negative type, then B is positive definite.*

3. The main results. The main contributions of the paper will be described in three steps. In the first one, we propose a result that extends the following property: if $g : Y \times Y \to (0, \infty)$ belongs to $CND_1(Y)$ and $\alpha > 0$, then $(y, y') \in Y \times Y \mapsto g(y, y')^{-\alpha}$ belongs to $PD_1(Y)$. Further, if $g(y, y) + g(y', y') - 2g(y, y') < 0$, for $y \neq y'$, then $(y, y') \in Y \times Y \mapsto g(y, y')^{-\alpha}$ belongs to $SPD_1(Y)$. This property follows from a few facts combined: $t \in (0, \infty) \mapsto t^{-\alpha}$ is completely monotone, with integral representation according to Bernstein-Widder Theorem ([26, p.3]) given by ([11, p.346])

$$\frac{1}{t^\alpha} = \frac{1}{\Gamma(\alpha)} \int_0^\infty e^{-ts} s^{\alpha-1} ds, \quad t > 0, \tag{3.3}$$

and Lemma2.3-$(i) - (ii)$.

THEOREM 3.1. *Let $G : Y \times Y \to M_q(\mathbb{R})$ be a matrix function in $CND_q(Y)$. Assume the range of G contains positive definite matrices only. If $m \in \mathbb{Z}_+ \setminus \{0\}$, then the following assertions hold for the kernel K_m defined by*

$$K_m(y, y') = \frac{1}{[\det G(y, y')]^{m/2}}, \quad y, y' \in Y.$$

(*i*) *K_m belongs to $PD_1(Y)$.*
(*ii*) *If there exists $u_0 \in \mathbb{R}^q \setminus \{0\}$ so that*

$$u_0^{\intercal}[G(y, y) + G(y', y') - 2G(y, y')]u_0 < 0, \quad y \neq y',$$

then K_m belongs to $SPD_1(Y)$.

Proof. Since every matrix $G(y, y')$ is invertible, K_1 is well-defined. We apply Lemma 2.2 to write

$$K_1(y, y') = \frac{1}{\pi^{q/2}} \int_{\mathbb{R}^q} e^{-u^{\intercal} G(y,y') u} du, \quad y, y' \in Y.$$

If $n \geq 1$, $y_1, \ldots, y_n$ are distinct points in Y and $c_1, \ldots, c_n$ are real numbers, then

$$\sum_{\mu,\nu=1}^{n} c_\mu^\intercal c_\nu K_1(y_\mu, y_\nu) = \frac{1}{\pi^{q/2}} \int_{\mathbb{R}^q} \sum_{\mu,\nu=1}^{n} c_\mu c_\nu e^{-u^\intercal G(y_\mu, y_\nu) u} du.$$

Lemma 2.1-(i) asserts that the kernels $(y, y') \in Y \times Y \mapsto u^\intercal G(y, y')u$, $u \in \mathbb{R}^q$, belong to $CND_1(Y)$ while Lemma 2.3-(i) reveals that

$$\sum_{\mu,\nu=1}^{n} c_\mu\, c_\nu e^{-u^\intercal G(y_\mu, y_\nu) u} \geq 0, \quad u \in \mathbb{R}^q.$$

Thus, $K_1 \in PD_1(Y)$. That the same property holds for the kernels K_m when $m \in \{2, 3, \ldots\}$, is a direct consequence of the Schur product Theorem ([9, p.477]). Therefore, Assertion (i) is proved.
In order to prove (ii) fix $n \geq 1$, the y_μ and the c_μ as before, with the c_μ not all zero. If there exists $u_0 \in \mathbb{R}^q \setminus \{0\}$ so that $u_0^\intercal[G(y, y) + G(y', y') - 2G(y, y')]u_0 < 0$, for $y \neq y'$, then Lemma 2.3-(ii) implies that

$$\sum_{\mu,\nu=1}^{n} c_\mu\, c_\nu e^{-u_0^\intercal G(y_\mu, y_\nu) u_0} > 0.$$

Since

$$u \in \mathbb{R}^q \mapsto \sum_{\mu,\nu=1}^{n} c_\mu\, c_\nu e^{-u^\intercal G(y_\mu, y_\nu) u}$$

is continuous, there is an open set U of $\mathbb{R}^q$ that contains u_0 so that

$$\sum_{\mu,\nu=1}^{n} c_\mu\, c_\nu e^{-u^\intercal G(y_\mu, y_\nu) u} > 0, \quad u \in U.$$

In particular,

$$\int_{\mathbb{R}^q} \sum_{\mu,\nu=1}^{n} c_\mu\, c_\nu e^{-u^\intercal G(y_\mu, y_\nu) u} du > 0,$$

that is, $\sum_{\mu,\nu=1}^{n} c_\mu\, c_\nu K_1(y_\mu, y_\nu) > 0$. It is now clear that $K_1 \in SPD_1(Y)$. The inequality $\det G(y, y) > 0$, for $y \in Y$, along with Oppenheim's inequality ([9, p.509]) justify that K_m belongs to $SPD_1(Y)$ when $m \geq 2$. □

It is an open question whether the positive definiteness of K_m in Theorem 3.1-(i) remains when the power $m/2$ in its definition is replaced with a real number $\alpha \geq 1/2$.

REMARK 3.2. *We do not know of any specific method that allows one to obtain from a fixed matrix kernel $G : Y \times Y \to M_q(\mathbb{R})$ in $CND_q(Y)$ another one of the same type but with range containing positive definite matrices only. However, depending on the setting, the addition of a convenient positive definite matrix to G will produce that effect.*

REMARK 3.3. *The assumption on G in Theorem 3.1-(ii) is always granted whenever the kernel G belongs to $SCND_q(Y)$. Indeed, Lemma 2.1 and Lemma 2.3-(iii)*

imply that $u^{\intercal}[G(y,y)+G(y',y')-2G(y,y')]u<0$, *for* $y\neq y'$ *and* $u\in\mathbb{R}^q\setminus\{0\}$, *whenever* G *belongs to* $SCND_q(Y)$.

EXAMPLE 3.4. We will consider continuous radial kernels on $Y=\mathbb{R}^d$, that is, radial matrix kernels $G:Y\times Y\to M_q(\mathbb{R})$ of the form

$$G(y,y')=g(\|y-y'\|),\quad y,y'\in Y,$$

where $g:[0,\infty)\to M_q(\mathbb{R})$ is continuous. According to Theorem 4.1 in [12], G as above belongs to $SCND_q(Y)$ if and only if

$$g(t)=\left[-\sum_{m=0}^{1}a_{\mu\nu}^{m}t^{2m}-\int_{(0,\infty)}\Omega_{1,d}(r,t)d\sigma_{\mu\nu}(r)\right]_{\mu,\nu=1}^{q},$$

in which the matrices $[a_{\mu\nu}^m]_{\mu,\nu=1}^q$, $m=0,1$, are symmetric, the matrix $[-a_{\mu\nu}]_{\mu\nu=1}^q$ is positive semi-definite, $\{\sigma_{\mu\nu}:\mu,\nu=1,\ldots,q\}$ is a family of signed measures on $(0,\infty)$, and the measure $\sum_{\mu,\nu=1}^q c_\mu c_\nu\sigma_{\mu\nu}$ is nonzero and positive whenever the real numbers $c_1,\ldots,c_q$ are not all zero. The function $\Omega_{1,d}$ is calculated through the formula

$$\Omega_{1,d}(r,t)=\frac{\Omega_d(rt)-e^{-r^2}}{\min\{1,r^2\}},$$

where the radial function $y\in Y\mapsto\Omega_d(y)=\Omega_d(\|y\|)$ is given by the mean-value of $x\in S^{d-1}\mapsto\exp(iy^{\intercal}x)$ over the unit sphere S^{d-1} of Y. If one can choose a positive definite matrix C so that $C+G(y,y')$ is a positive definite matrix of $M_q(\mathbb{R})$ for $y,y'\in Y$, then Theorem 3.1 is applicable for $C+G$.

EXAMPLE 3.5. Here we will let Y be the unit sphere S^d in $\mathbb{R}^{d+1}$ endowed with its usual geodesic distance δ_d. Every function of the form

$$g(t)=g(0)+\sum_{k=1}^{\infty}A_k\left[1-p_k^d(t)\right],\quad t\in[0,\pi],$$

where each A_k is a positive semi-definite element of $M_q(\mathbb{R})$, the series $\sum_{k=1}^\infty A_k$ is convergent and p_k^d denotes the Gegenbauer polynomial of degree k associated with the rational $(d-1)/2$ so normalized that $p_k^d(1)=1$, induces a kernel

$$(y,y')\in S^d\times S^d\mapsto G(y,y'):=g(\delta_d(y,y'))$$

in $CND_q(S^d)$ and vice-versa ([6]). Taking into account that the diagonal functions in the series representation for G belong to $CND_1(S^d)$ and that g is bounded, we can pick a positive definite matrix P in $M_d(\mathbb{R})$ so that $P+G(y,y')$ is positive definite for all $y,y'\in S^d$. The kernel K_m in Theorem 3.1 belongs to $PD_q(S^d)$ as long as we replace G with its perturbed version $P+G$. It is easy to see that if $d>1$ and A_k is nonzero for one odd k, then

$$\sum_{k=1}^{\infty}\left[1-p_k^d(\delta_d(y,y'))\right]u^{\intercal}A_ku>0 \tag{3.4}$$

whenever $u\notin\ker A_k$ and $y\neq y'$, that is, $u^{\intercal}[G(y,y)+G(y',y')-2G(y,y')]u<0$ for $u\notin\ker A_k$ and $y\neq y'$. Therefore, K_m belongs to $SPD_q(S^d)$ if (3.4) holds. This example can be extrapolated to the case in which Y is the unit sphere in the real ℓ_2 endowed with its natural distance after we replace p_k^d with $p_k^\infty(t) := t^k$ in the previous arguments.

Theorem 3.8 below is a generalization of Theorem 3.1, after the introduction of completely monotone functions into the setting. Prior to that, we find it convenient to introduce the notion we call exponential positive definiteness.

A vector function $H : X \times X \to \mathbb{C}^q$ is said to be *exponentially positive definite* on X if all the exponentials

$$(x, x') \in X \times X \mapsto e^{i\,H(x,x')^* u}, \quad u \in \mathbb{R}^q,$$

belong to $PD_1(X)$. Since a kernel in $PD_1(X)$ is necessarily Hermitian, direct computation reveals that a necessary condition in order that a vector function H is exponentially positive definite is that its real part is anti-symmetric in the sense that

$$\operatorname{Re} H(x, x') = -\operatorname{Re} H(x', x), \quad x, x' \in X.$$

In particular, if $H : X \times X \to \mathbb{R}^q$ is exponentially positive definite, then $H(x, x) = 0$, $x \in X$. It is very easy to verify that a kernel H is exponentially positive definite if and only if the kernel sH is so for $s > 0$.

A less obvious necessary condition for the exponential positive definiteness of a vector function is provided by the proposition below.

PROPOSITION 3.6. *If a vector function $H : X \times X \to \mathbb{R}^q$ is exponentially positive definite, then $(x, x') \in X \times X \mapsto \|H(x, x')\|^2$ belongs to $CND_1(X)$.*

Proof. If we write $b = 2\sqrt{s}\, H(x, x')$, $s > 0$, and let A be the identity matrix of order q in Lemma 2.2, we obtain

$$e^{-s\|H(x,x')\|^2} = \frac{1}{\pi^{q/2}} \int_{\mathbb{R}^q} e^{-u^\intercal u + i\,2\sqrt{s}\ H(x,x')^\intercal u} du, \quad x, x' \in X.$$

Since $2\sqrt{s}\ H$ is exponentially positive definite and the measure μ given by $d\mu(u) = e^{-u^\intercal u} du$ is finite and positive, it follows that all the kernels

$$(x, x') \in X \times X \mapsto e^{-s\|H(x,x')\|^2}, \quad s > 0,$$

belong to $PD_1(X)$. However, Theorem 2.2 in [3] shows that the kernel $(x, x') \in X \times X \mapsto \|H(x, x')\|^2$ must belong to $CND_1(X)$. □

Proposition 3.6 suggests the following class of examples.

EXAMPLE 3.7. For any function $h : X \to \mathbb{R}^q$, the formula

$$H(x, x') = h(x) - h(x'), \quad x, x' \in X,$$

defines an exponentially positive definite vector function H on X.

We do not know if Example 3.7 exhausts the class of exponentially positive definite vector functions with range in $\mathbb{R}^q$.

THEOREM 3.8. *Let $\phi : (0, \infty) \to \mathbb{R}$ be a bounded and completely monotone function, $G : Y \times Y \to M_q(\mathbb{R})$ a matrix function in $CND_q(Y)$, and $H : Y \times Y \to \mathbb{R}^q$ an exponentially positive definite vector function. Assume the range of G contains* *positive definite matrices only. If $m \in \mathbb{Z}_+ \setminus \{0\}$, then the following assertions hold for the kernel K_m given by the formula*

$$K_m(y,y') = \frac{\phi\left(H(y,y')^\intercal G(y,y')^{-1} H(y,y')\right)}{[\det G(y,y')]^{m/2}}, \quad y,y' \in Y.$$

(i) K_m belongs to $PD_1(Y)$.
(ii) If ϕ is not identically zero and there exists u_0 in $\mathbb{R}^q$ so that

$$u_0^\intercal [G(y,y) + G(y',y') - 2G(y,y')] u_0 < 0, \quad y \neq y',$$

then K_m belongs to $SPD_1(Y)$.

Proof. In view of the proof of Theorem 3.1, it suffices to prove the theorem in the case where $m = 1$. The Bernstein-Widder Theorem provides the integral representation for ϕ in the form

$$\phi(t) = \int_{[0,\infty)} e^{-t\,s} d\sigma(s), \quad t \geq 0,$$

where σ is a finite positive measure on $[0,\infty)$ and it implies that

$$K_1(y,y') = \frac{1}{[\det G(y,y')]^{1/2}} \int_{[0,\infty)} e^{-H(y,y')^\intercal G(y,y')^{-1} H(y,y')\,s} d\sigma(s), \quad y,y' \in Y.$$

After an application of Lemma 2.2, we can write

$$K_1(y,y') = \frac{1}{\pi^{q/2}} \int_{[0,\infty)} \left[\int_{\mathbb{R}^q} e^{-u^\intercal G(y,y')u + i\,2\sqrt{s}\,H(y,y')^\intercal u} du \right] d\sigma(s), \quad y,y' \in Y.$$

If $n \geq 1$, $y_1, \ldots, y_n$ are distinct points in Y and $c_1, \ldots, c_n$ are complex numbers, then

$$\sum_{\mu,\nu=1}^{n} \overline{c_\mu}\, c_\nu K_1(y_\mu, y_\nu) = \frac{1}{\pi^{q/2}} \int_{[0,\infty)} \left[\int_{\mathbb{R}^q} \sum_{\mu,\nu=1}^{n} \overline{c_\mu}\, c_\nu A^u_{\mu\nu} B^{u,s}_{\mu\nu}\, du \right] d\sigma(s),$$

where

$$A^u_{\mu\nu} = e^{-u^\intercal G(y_\mu,y_\nu)u}, \quad \mu,\nu = 1,\ldots,n;\ u \in \mathbb{R}^q$$

and

$$B^{u,s}_{\mu\nu} = e^{i\,2\sqrt{s}\,H(y_\mu,y_\nu)^\intercal u}, \quad \mu,\nu = 1,\ldots,n;\ u \in \mathbb{R}^q;\ s > 0.$$

Each matrix $\left[A^u_{\mu\nu}\right]^n_{\mu,\nu=1}$ is positive semi-definite by Lemma 2.1-(i) and Lemma 2.3-(i) while each $[B^{u,s}_{\mu\nu}]^n_{\mu,\nu=1}$ is positive semi-definite by our assumption on H. Invoking the Schur Product Theorem, we can infer that

$$\sum_{\mu,\nu=1}^{n} \overline{c_\mu}\, c_\nu A^u_{\mu\nu} B^{u,s}_{\mu\nu} \geq 0, \quad u \in \mathbb{R}^q;\ s \geq 0.$$

Thus, $\sum_{\mu,\nu=1}^n \overline{c_\mu}\, c_\nu K_1(y_\mu,y_\nu) \geq 0$ and $K_1 \in PD_1(Y)$.

In order to ratify (ii), let the y_μ and the c_μ be as before with the c_μ not all zero. We will assume ϕ is not identically zero and the existence of u_0 in $\mathbb{R}^q$ so that

$u_0^\intercal[G(y,y)+G(y',y')-2G(y,y')]u_0<0$, for $y\neq y'$ and will proceed considering two cases. If σ is concentrated at zero, then $K_1(y,y')=C[\det G(y,y')]^{-1/2}$, for some $C>0$ and we can apply Theorem 3.1-(ii) in order to see that $\sum_{\mu,\nu=1}^n \overline{c_\mu}\, c_\nu K_1(y_\mu,y_\nu)>0$. If σ is not concentrated at 0, the proof of Theorem 3.1 allows us to assume the existence of an open subset U of $\mathbb{R}^q$ containing u_0 so that

$$\sum_{\mu,\nu=1}^n \overline{c_\mu} c_\nu A^u_{\mu,\nu}>0, \quad u\in U.$$

Since the diagonal elements of the positive semi-definite matrices $B^{u,s}$ are all positive, Oppenheim's inequality shows that actually

$$\sum_{\mu,\nu=1}^n \overline{c_\mu}\, c_\nu A^u_{\mu\nu} B^{u,s}_{\mu\nu}>0, \quad u\in U;\ s\geq 0,$$

and, consequently,

$$\int_{\mathbb{R}^q}\sum_{\mu,\nu=1}^n \overline{c_\mu}\, c_\nu A^u_{\mu\nu} B^{u,s}_{\mu\nu} du>0, \quad s\geq 0.$$

Recalling the assumption on σ, it is now clear that

$$\int_{[0,\infty)}\left(\int_{\mathbb{R}^q}\sum_{\mu,\nu=1}^n \overline{c_\mu}\, c_\nu A^u_{\mu\nu} B^{u,s}_{\mu\nu} du\right) d\sigma(s)>0.$$

In both cases, we can conclude that $K_1\in SPD_1(Y)$, and (ii) is proved. □

Theorem 5 in [23] is a particular case of Theorem 3.8-(i). The current approach and proof are completely different.

Example 3.9. If g is a function with domain Y and range in the set of all $l\times q$ real matrices, then $(y,y')\in Y\times Y\mapsto -g(y)^\intercal g(y')$ belongs to $CND_q(\mathbb{R})$. Assume there exists a positive semi-definite matrix A in $M_q(\mathbb{R}^q)$ so that $G(y,y')=A-g(y)^\intercal g(y')$ is positive definite for all y and y' in Y. According to Theorem 3.8, if $h:Y\to\mathbb{R}^q$ is an arbitrary function, then the kernel $K_m: Y\times Y\to\mathbb{R}$ given by

$$K_m(y,y')=\frac{[1+c(h(y)-h(y'))^\intercal G(y,y')^{-1}(h(y)-h(y'))]^{-\nu}}{[\det G(y,y')]^{m/2}}$$

belongs to $PD_1(Y)$ whenever $c,\nu>0$ and $m\geq 1$.

Example 3.10. Keeping h as in Example 3.9, if $\mathcal{M}_\nu$ is the normalized Matérn function given by

$$\mathcal{M}_\nu(u)=\frac{2^{1-\nu}}{\Gamma(\nu)}u^\nu\mathcal{K}_\nu(u), \quad u\geq 0,$$

where Γ stands for the usual Gamma function, $\mathcal{K}_\nu$ is the modified Bessel function of second kind, and $\nu>0$, then the same is true of

$$K_m(y,y')=\frac{\mathcal{M}_\nu(c[(h(y)-h(y'))^\intercal G(y,y')^{-1}(h(y)-h(y'))]^{1/2})}{[\det G(y,y')]^{m/2}}$$

whenever $c > 0$ and $m \geq 1$.

EXAMPLE 3.11. If we define $G : Y \times Y \to \mathbb{R}^q$ through the formula $G(y, y') = g(y, y')I_q$, $y, y' \in Y$, where I_q denotes the identity matrix of order q and $g : Y \times Y \to (0, \infty)$ is a kernel in $CND_1(Y)$, then G belongs to $CND_q(Y)$. It is easily seen that $G(y, y')$ is positive definite for all $y, y' \in Y$. Thus, if ϕ is a bounded and completely monotone function and $H : X \times X \to \mathbb{R}^q$ is an exponentially positive definite function, an application of Theorem 3.8 shows that the formula

$$K_m(y, y') = \frac{1}{g(y, y')^{mq/2}} \phi\left(\frac{\|H(y, y')\|^2}{g(y, y')}\right), \quad y, y' \in Y,$$

defines a kernel in $PD_1(Y)$ whenever $m \in \mathbb{Z}_+ \setminus \{0\}$. However, observing that $(y, y') \in Y \times Y \mapsto g(y, y')^{-\alpha}$, $\alpha \in (0, \infty)$, belongs to $PD_1(Y)$, the Schur Product Theorem yields that the same is true for K_m with $m \in [q, \infty)$. If $g(y, y) + g(y', y') - 2g(y, y') < 0$ when $y \neq y'$, we may infer from Theorem 3.8-(ii) that $K_m \in SPD_1(Y)$ as long as ϕ is nonconstant.

Next, we move to a generalization of Theorem 3.8 motivated by results we found in the statistical literature (for instance, see the construction in [7]). The result is also suggested by the first integral formula for K_1 appearing in the proof of Theorem 3.8.

THEOREM 3.12. *Let ρ be a nonzero positive measure on $(0, \infty)$, ϕ a bounded completely monotone function and $\{P_s\}_{s>0}$ a family of kernels in $PD_1(Y)$ such that each function $s \in (0, \infty) \mapsto P_s(y, y')$ is ρ-integrable. If G and H are as in Theorem 3.8, then the following assertions hold for the kernel $K_m : Y \times Y \to \mathbb{C}$, $m \in \mathbb{Z}_+ \setminus \{0\}$, given by the formula*

$$K_m(y, y') = \frac{1}{[\det G(y, y')]^{m/2}} \int_{(0,\infty)} \phi(H(y, y')^\intercal G(y, y')^{-1} H(y, y') s) P_s(y, y') d\rho(s).$$

- (i) *K_m belongs to $PD_1(Y)$.*
- (ii) *If ϕ is not identically zero and there exist u_0 in $\mathbb{R}^q$ so that*
$$u_0^\intercal [G(y, y) + G(y', y') - 2G(y, y')] u_0 < 0, \quad y \neq y',$$
and a ρ-measurable subset A of $(0, \infty)$ so that $\rho(A) > 0$ and $P_s(y, y) > 0$, $y \in Y$, $s \in A$, then K_m belongs to $SPD_1(Y)$.
- (iii) *If ϕ is not identically zero and there exists a ρ-measurable subset A of $(0, \infty)$ so that $\rho(A) > 0$ and P_s belongs to $SPD_1(Y)$, for $s \in A$, then K_m belongs to $SPD_1(Y)$.*

Proof. As before, it suffices to prove the theorem in the case where $m = 1$. First observe that

$$K_1(y, y') = \int_{(0,\infty)} \frac{1}{[\det G(y, y')]^{1/2}} \phi(\sqrt{s}\, H(y, y')^\intercal G(y, y')^{-1} \sqrt{s}\, H(y, y')) P_s(y, y') d\rho(s).$$

Hence, by Theorem 3.8-(i), the integrand in the expression above is a product of kernels in $PD_1(Y)$, for all $s > 0$. Therefore, Assertion (i) follows from the Schur Product Theorem.

To proceed, assume ϕ is not identically zero and let n, the y_μ and the c_μ be as in the proof of Theorem 3.8, with the c_μ not all zero. If there exists u_0 as described in (ii), we may apply Theorem 3.8-(ii) in order to see that the kernels

$$(y, y') \in Y \times Y \mapsto \frac{\phi(\sqrt{s}\, H(y, y')^\intercal G(y, y')^{-1} \sqrt{s}\, H(y, y'))}{[\det G(y, y')]^{1/2}}, \quad s > 0,$$

belong to $SPD_1(Y)$. But, if there is a ρ-measurable subset A of $(0,\infty)$ so that $\rho(A) > 0$ and $P_s(y,y) > 0$, $y \in Y$, $s \in A$, then Oppenheim's inequality implies that the kernels

$$(y,y') \in Y \times Y \mapsto \frac{\phi(\sqrt{s}\, H(y,y')^\intercal G(y,y')^{-1} \sqrt{s}\, H(y,y'))P_s(y,y')}{[\det G(y,y')]^{1/2}}, \quad s \in A,$$

belong to $SPD_1(Y)$ as well. Thus, Assertion (ii) follows. Assertion (iii) is again a consequence of Oppenheim's inequality and the equality $H(y,y) = 0$, $y \in Y$. □

REMARK 3.13. *It is straightforward to verify that Theorem 3.12 also holds for the model*

$$K_m(y,y') = \frac{1}{[\det G(y,y')]^{m/2}} \int_{(0,\infty)} \phi(H(y,y')^\intercal G(y,y')^{-1} H(y,y') h(s)) P_s(y,y') d\rho(s),$$

whenever $h : (0,\infty) \to (0,\infty)$ *is a function for which*

$$s \in (0,\infty) \mapsto \phi(H(y,y')^\intercal G(y,y')^{-1} H(y,y') h(s)) P_s(y,y')$$

is ρ*-integrable.*

4. Applications. In this section we present some specific models that serve as either examples or applications of Theorem 3.12. Some of them are abstract versions of models previously discussed in restricted settings in the literature.

A model based on the negative power function: We make use of the integral formula (3.3) in order to deduce the equality

$$\int_{(0,\infty)} e^{-us}(a+bs)d\rho(s) = \sqrt{\pi}\left(\frac{a}{\sqrt{u+a}} + \frac{b}{2\sqrt{(u+a)^3}}\right), \quad u \geq 0,$$

where $a, b > 0$ and $d\rho(s) = e^{-as}s^{-1/2}ds$. If we set $\phi(u) = e^{-u}$, $u > 0$ and

$$P_s(y,y') = Q(y,y') + 2sR(y,y'), \quad y, y' \in Y,$$

in which $Q, R \in PD_1(Y)$, then Theorem 3.12-(i) implies that

$$K_m(y,y') = \frac{1}{[\det G(y,y')]^{m/2}} \left[\frac{Q(y,y')}{\sqrt{H(y,y')^\intercal G(y,y')^{-1} H(y,y') + Q(y,y')}} \right.$$
$$\left. + \frac{R(y,y')}{\sqrt{(H(y,y')^\intercal G(y,y')^{-1} H(y,y') + Q(y,y'))^3}} \right], \quad y, y' \in Y,$$

belongs to $PD_1(Y)$ as long as G and H satisfy the assumptions of that theorem. On the other hand, Theorem 3.12-(ii) implies that K_m actually belongs to $SPD_1(Y)$ whenever ϕ is not identically 0, there exists u_0 in $\mathbb{R}^q$ so that $u_0^\intercal[G(y,y) + G(y',y') - 2G(y,y')]u_0 < 0$ for $y \neq y'$, and $Q(y,y) + sR(y,y) > 0$ for $y \in Y$ and $s \in A$, where A is ρ-measurable and $\rho(A) > 0$. The same conclusion can be reached if ϕ is not identically 0 and $Q + sR$ belongs to $SPD_1(Y)$ for $s \in A$, where A is as before.

A model based on the generalized Cauchy function: Here, we will make use of the following well-known integral representation for the generalized Cauchy function ([11, p.337])

$$\frac{1}{(\beta+cu^\gamma)^\nu}=\frac{c^{-\nu}}{\Gamma(\nu)}\int_0^\infty e^{-s\,u^\gamma}s^\nu d\rho(s),\quad u\geq 0,$$

where $\beta>0$, $\nu>1$, $\gamma\in(0,1]$, and $d\rho(s)=s^{-1}\exp(-\beta\, s/c)$. Setting $\phi(u)=e^{-u^\gamma}$, $u>0$ and

$$P_s(y,y')=\left(\frac{s}{c}\right)^{v(y)+v(y')},\quad s>0;\ y,y'\in Y,$$

where $v:Y\to(0,\infty)$ is chosen in such a way that $s\in(0,\infty)\mapsto s^{v(y)}$ is ρ-integrable for each $y\in Y$, Theorem 3.12 implies that the model

$$K_m(y,y')=\frac{\Gamma(v(y)+v(y'))}{[\det G(y,y')]^{m/2}}\left[\beta+c(H(y,y')^\intercal G(y,y')^{-1}H(y,y'))^\gamma\right]^{-v(y)-v(y')},$$

belongs to $PD_1(Y)$ as long as G and H satisfy the assumptions of the theorem. If one takes $Y=\mathbb{R}^q$, $H(y,y')=y-y'$, $y,y'\in Y$, $c=\gamma=1$, then the model

$$S_m(y,y')=\frac{\Gamma(v(y)+v(y'))}{[\det G(y,y')]^{m/2}}\left[\beta+(y-y')^\intercal G(y,y')^{-1}(y-y')\right]^{-v(y)-v(y')},\quad y,y'\in Y,$$

belongs to $PD_1(Y)$ if we keep the assumptions of Theorem 3.12 on G. This model is close to another one discussed in [25]. Some other theorems and examples aligned with this reference can be either reformulated or deduced from assertions made in the theorems proved in this paper. For instance, that is the case in some results discussed in [16, 19].

A model with the parabolic cylinder function: This example begins with the formula ([11, p.365])

$$\Gamma(\nu)e^{u^2/4}D_{-\nu}(u)=\int_0^\infty e^{-u\,s}s^\nu d\rho(s),\quad u\geq 0,$$

where $D_{-\nu}$ is the parabolic cylinder function with index $\nu>0$ and $d\rho(s)=s^{-1}\exp(-s^2/2)$. Setting $\phi(u)=e^{-u}$, $u>0$ and

$$P_s(y,y')=s^{v(y)+v(y')},\quad s>0;\ y,y'\in Y,$$

where $v:Y\to(0,\infty)$ is chosen in such a way that $s\in(0,\infty)\mapsto s^{v(y)}$ is ρ-integrable for each $y\in Y$, an application of Theorem 3.12 shows that

$$K_m(y,y')=\frac{\Gamma(v(y)+v(y'))}{[\det G(y,y')]^{m/2}}\,e^{(H(y,y')^\intercal G(y,y')^{-1}H(y,y'))^2/4}\times D_{-v(y)-v(y')}(H(y,y')^\intercal G(y,y')^{-1}H(y,y')),\quad y,y'\in Y,$$

belongs to $PD_1(Y)$, as long as G and H satisfy the assumptions of the theorem.

A model with the Matérn function: We will employ the formula ([4])

$$\mathcal{M}_\nu(\sqrt{u})=\frac{1}{4^\nu\Gamma(\nu)}\int_0^\infty e^{-s\,u}e^{-1/4s}s^{-\nu-1}ds,\quad u>0.$$

Setting $\phi(u) = \exp(-u)$, $u > 0$, $d\rho(s) = e^{-1/4s}s^{-1}$, and $\{P_s\}_{s>0}$ as in the previous example, an application of Theorem 3.12 shows that B_m given by

$$B_m(y,y') = \frac{\Gamma(v(y)+v(y'))}{[\det G(y,y')]^{m/2}}\mathcal{M}_{v(y)+v(y')}((H(y,y')^{\intercal}G(y,y')^{-1}H(y,y'))^{1/2}), \quad y,y' \in Y,$$

belongs to $PD_1(Y)$ whenever G and H fit the assumptions of that theorem. If we set $G(y,y') = g(y,y')I_q$, where g is a positive valued kernel in $CND_1(Y)$, then B_m takes the form

$$B_m(y,y') = \frac{\Gamma(v(y)+v(y'))}{g(y,y')^{qm/2}}\mathcal{M}_{v(y)+v(y')}\left(\frac{\|H(y,y')\|}{g(y,y')^{1/2}}\right), \quad y,y' \in Y.$$

Observe that the B_m above actually belongs to $SPD_1(Y)$ whenever $g(y,y) + g(y',y') - 2g(y,y') < 0$ for $y \neq y'$.

The analysis of the strict positive definiteness in some of the examples above was compromised because either we did not specify G or we could not guarantee the strict positive definiteness of the P_s chosen.

5. Extensions to positive definiteness on products. In this section we explain how to adapt Theorems 3.8 and 3.12 in order to cover positive definiteness on a product $X \times Y$ of sets. The results can be applied in the construction of covariance functions associated with random processes for space-time models.

Let us begin with an extension of Theorem 3.8.

THEOREM 5.1. *Let $\phi : (0,\infty) \to \mathbb{R}$ be a bounded and completely monotone function, $G : Y \times Y \to M_q(\mathbb{R})$ a matrix function in $CND_q(Y)$, and $H : X \times X \to \mathbb{R}^q$ an exponentially positive definite function. Assume the range of G contains positive definite matrices only. If $m \in \mathbb{Z}_+$, then the kernels $K_m : (X \times Y)^2 \to \mathbb{R}$ given by*

$$K_m((x,y),(x',y')) = \frac{\phi\left(H(x,x')^{\intercal}G(y,y')^{-1}H(x,x')\right)}{[\det G(y,y')]^{m/2}},$$

belong to $PD_1(X \times Y)$.

Proof. It suffices to follow the arguments in the first half of the proof of Theorem 3.8. If $n \geq 1$, $(x_1,y_1),\ldots,(x_n,y_n)$ are distinct points in $X \times Y$ and $c_1,\ldots,c_n$ are complex numbers, then

$$\sum_{\mu,\nu=1}^{n} \overline{c_\mu}\, c_\nu K_1((x_\mu,y_\mu),(x_\nu,y_\nu)) = \frac{1}{\pi^{q/2}}\int_{[0,\infty)}\int_{\mathbb{R}^q}\sum_{\mu,\nu=1}^{n} \overline{c_\mu}\, c_\nu A_{\mu\nu}^{u} B_{\mu\nu}^{u,s}\, du d\sigma(s),$$

where

$$A_{\mu\nu}^{u} = e^{-u^{\intercal}G(y_\mu,y_\nu)u}, \quad \mu,\nu = 1,\ldots,n,$$

and

$$B_{\mu\nu}^{u,s} = e^{i\,2H(x_\mu,x_\nu)^{\intercal}u\sqrt{s}}, \quad \mu,\nu = 1,\ldots,n.$$

As before, the matrices $\left[A_{\mu\nu}^{u}\right]_{\mu,\nu=1}^{n}$ are positive semi-definite by Lemma 2.1-(i) and Lemma 2.3-(i) while the $[B_{\mu\nu}^{u,s}]_{\mu,\nu=1}^{n}$ are positive semi-definite by our assumption on H. So, the Schur Product Theorem once again substantiates that

$$\sum_{\mu,\nu=1}^{n} \overline{c_\mu}\, c_\nu K_1((x_\mu,y_\mu),(x_\nu,y_\nu)) \geq 0.$$

In particular, K_1 is positive definite. The result follows. □

Theorem 5.1 leads to the following abstract generalization of Gneiting's original criterion proved in [8]. Its proof can be adapted from the arguments developed in Example 3.9.

THEOREM 5.2. *Let $\phi : (0,\infty) \to \mathbb{R}$ be a bounded and completely monotone function, $g : Y \times Y \to (0,\infty)$ a kernel in $CND_1(Y)$, and $H : X \times X \to \mathbb{R}^q$ an exponentially positive definite function. If $r \geq q$, then the kernel $K_r : (X \times Y)^2 \to \mathbb{R}$ given by*

$$K_r((x,y),(x',y')) = \frac{1}{g(y,y')^{r/2}}\phi\left(\frac{\|H(x,x')\|^2}{g(y,y')}\right), \quad x,x' \in X;\ y,y' \in Y,$$

belongs to $PD_1(X \times Y)$.

REMARK 5.3. *Theorem 5.2 cannot be obtained by the Fourier techniques used by Gneiting in [8]. We also think that the alternative techniques used by other authors to prove some extensions of Gneiting's original result do not apply either. If we set $X = \mathbb{R}^q$, $H(x,x') = x - x'$, $x,x' \in X$, $Y = \mathbb{R}^d$, and $G(y,y') = g(\|y-y'\|^2)$, $y,y' \in Y$, where $g : (0,\infty) \to (0,\infty)$ is a function having a completely monotone derivative, Theorem 5.2 recovers the original Gneiting's model itself. We observe that, within this setting, Gneiting's model extends to the case in which $H(x,x') = h(x) - h(x')$, $x,x' \in X$, where $h : X \to \mathbb{R}^q$ is a given function.*

Next, we present a version of Theorem 3.12 to products but leave the proof to the interested reader.

THEOREM 5.4. *Let X, Y, ϕ, G and H be as in Theorem 5.1. Let ρ be a nonzero positive measure on $(0,\infty)$ and $\{P_s\}_{s>0}$ a family of kernels in $PD_1(X \times Y)$ so that each function $s \in (0,\infty) \mapsto P_s((x,y),(x',y'))$ is ρ-integrable. If $m \in \mathbb{Z}_+$, then the kernel K_m given by*

$$K_m((x,x'),(y,y')) = \frac{1}{[\det G(y,y')]^{m/2}}\int_{(0,\infty)} \phi(H(x,x')^{\intercal} G(y,y')^{-1} H(x,x')s) \times P_s((x,y),(x',y'))d\rho(s), \quad x,x' \in X;\ y,y' \in Y,$$

belongs to $PD_1(X \times Y)$.

REMARK 5.5. *For distinct points $(x_1,y_1),\ldots,(x_n,y_n)$ in $X \times Y$, the x-components and the y-components may be no longer distinct. Hence, the arguments used to prove strict positive definiteness in Theorems 3.8 and 3.12 no longer work to prove similar properties in Theorems 5.1 and 5.4.*

EXAMPLE 5.6. By borrowing notation and the arguments used in the model based on the negative power function described in Section 4, one may show that the model

$$K_m((x,x'),(y,y')) = \frac{1}{[\det G(y,y')]^{m/2}}\left[\frac{Q(x,x')}{\sqrt{H(x,x')^{\intercal} G(y,y')^{-1} H(x,x') + Q(x,x')}} + \frac{R(x,x')}{\sqrt{(H(x,x')^{\intercal} G(y,y')^{-1} H(x,x') + Q(x,x'))^3}}\right],$$

defines a kernel in $PD_1(X \times Y)$, as long as G and H are as in Theorem 5.4, and Q and R belong to $PD_1(X)$.

Acknowledgment. The authors are grateful to two anonymous referees for their valuable comments and suggestions.

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