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CONSTRUCTIVE APPROXIMATION

Interpolation of Scattered Data: Distance Matrices and Conditionally Positive Definite Functions

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Abstract. Among other things, we prove that multiquadric surface interpolation is always solvable, thereby settling a conjecture of R. Franke.

1. Introduction

For solving practical problems of data fitting in two dimensions, two methods seem to be most popular: *thin plate splines* (TPS) by Duchon [8] and Hardy's *multiquadric surfaces* (MQS) ([14, 15]; see also Franke [10]). The theory for TPS has been developed in a series of papers by Duchon [8] and Meinguet [21]. However, beyond its numerical performance, little seems to be known about the MQS method. For instance, in his lecture notes for a recent meeting, Franke [11] proposed (based on extensive numerical experience) the following conjecture:

Conjecture. Given any distinct points $x^1, \ldots, x^n$ in the plane

$$(1.1) \qquad (-1)^{n-1} \det \sqrt{1 + \|x^i - x^j\|^2} > 0,$$

where $\|x\|^2 = x_1^2 + x_2^2$, $x = (x_1, x_2)$, is the Euclidean norm of x.

This conjecture says, in particular, that there is a unique surface $f(x) = c_1\sqrt{1 + \|x - x^1\|^2} + \cdots + c_n\sqrt{1 + \|x - x^n\|^2}$ that interpolates (data) $y_1, \ldots, y_n$ at $x^1, \ldots, x^n$. Apparently, when this conjecture was made it was not even known that interpolation by MQS is always possible according to Wahba [29].

As an extension of MQS, Barnhill and Stead [5] explored surfaces based on the kernel $K_\mu(x, y) = (1 + \|x - y\|^2)^{-\mu}$, where μ is a real number, in contour plotting for three-dimensional interpolation. Thus they used

$$(1.2) \qquad f(x) = c_1 K_\mu(x, x^1) + \cdots + c_n K_\mu(x, x^n)$$

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to interpolate scattered data

$$f(x^i) = y_i, \qquad i = 1, \ldots, n, \tag{1.3}$$

and sought those values of μ for which (1.3) has a unique solution. A similar question was recently raised kernel $K(x, y) = \log(1 + \|x - y\|^2)$ by N. Dyn [9].

The purpose of this paper is to address these questions. We place them into a unified context so that we can draw upon ideas from the theory of positive definite functions by Stewart [28] and distance matrices by Blumenthal [6]. Therefore it is possible that some of what we say here may already be accessible in the literature.

2. Background and Results

Let X be an abstract point set. Suppose K is a real-valued kernel defined on $X \times X$ and $k_1(x), \ldots, k_m(x)$ are given real-valued functions over X. A sufficient condition that guarantees that the interpolation problem (1.3) has a solution of the form

$$f(x) = \sum_{i=1}^{n} c_i K(x, x^i) + \sum_{i=1}^{m} d_i k_i(x), \qquad m \le n, \tag{2.1}$$

that satisfies the auxiliary condition

$$\sum_{i=1}^{n} c_i k_j(x^i) = 0, \qquad j = 1, \ldots, m, \tag{2.2}$$

when rank $(k_i(x^j)) = m$ is that the quadratic form

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j K(x^i, x^j)$$

is strictly positive definite whenever $c = (c_1, \ldots, c_n)$ satisfies (2.2). The motivation for this type of interpolation comes from methods of *optimal interpolation*. Thus some quadratic seminorm can be introduced on a subspace of real-valued functions on X and the method (2.1), (2.2) will have the least norm among all solutions to (1.3). This equivalence is discussed by several authors (Matheron [19, 20], Salkauskas [23]). For instance, when $m = 0$, i.e., only the kernel K is present in (2.1), the construction of X can be based on Aronszajn's theory of reproducing kernels [3]. These matters are not of concern to us here. Rather, we are interested in *explicit* examples of (2.1), (2.2) which can be used to solve the scattered data interpolation problem in, for instance, two and three dimensions. For this purpose, we restrict $X = R^s$ and $K(x, y) = F(\|x - y\|^2)$, where F is a continuous real-valued function defined on $[0, \infty)$. Furthermore, we consider only the case where the span of $k_1(x), \ldots, k_m(x)$ is the space $\pi_{k-1}(R^s)$ of polynomials of total degree $\le k - 1$.

Definition 2.1. *A continuous function $F(t)$, defined on $[0, \infty)$, is said to be conditionally (strictly) positive definite of order k on R^s if for any distinct points*

$x^1, \ldots, x^n \in R^s$ and scalars $c_1, \ldots, c_n$ such that

$$\sum_{i=1}^{n} c_i p(x^i) = 0 \tag{2.3}$$

for all $p \in \pi_{k-1}(R^s)$, the quadratic form $\sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j F(\|x^i - x^j\|^2)$ is (positive) nonnegative.

We will denote the class of conditionally positive definite functions by $\mathscr{P}_k(R^s)$. Obviously, $\mathscr{P}_{k+1}(R^s) \subseteq \mathscr{P}_k(R^s)$.

A famous theorem of Bochner characterizes any $f(x) = F(\|x\|^2)$, $F \in \mathscr{P}_0(R^s)$ as the Fourier transform of a finite Borel measure on R^s (see Stewart [28]). Because $f(x)$ is a radial function this result has an equivalent formulation expressing $F(t)$ as a certain Bessel transform of a measure on R^1. Specifically,

$$F(t) = \int_0^\infty \Omega_s(tu)\, d\alpha(u),$$

where $\alpha(u)$ is bounded and nondecreasing, and Ω_s is defined by Schoenberg [26, 27] in terms of Bessel functions as

$$\Omega_s(t) = \begin{cases} \cos t, & s = 1, \\ \Gamma\left(\frac{s}{2}\right)\left(\frac{2}{t}\right)^{(s-2)/2} J_{(s-2)/2}(t), & s \geq 2. \end{cases}$$

Similar characterizations are available for the class $\mathscr{P}_k(R^s)$ [13, Chapter II].

We are especially interested in the class of functions that are conditionally positive definite of order k over any R^s, i.e.,

$$\mathscr{P}_k = \bigcap_{s \geq 1} \mathscr{P}_k(R^s). \tag{2.4}$$

To state our result about $\mathscr{P}_k$ we recall that a function F is said to be completely monotonic on $(0, \infty)$ provided that it is in $C^\infty(0, \infty)$ and $(-1)^l F^{(l)}(x) \geq 0$, $x \in (0, \infty)$, $l = 0, 1, 2, \ldots$.

Theorem 2.1. *$F \in \mathscr{P}_k$ whenever F is continuous on $[0, \infty)$ and $(-1)^k F^{(k)}$ is completely monotonic on $(0, \infty)$.*

The case $k = 0$ of this theorem is due to Schoenberg [27]. He even showed the equivalence of these conditions in this case. The general case and its elementary proof embody the TPS and MQS interpolation methods and lead us to a proof of (1.1).

Another result of this type is

Theorem 2.2. *Let $l = [s/2] - k + 2$ be a positive integer. Then for any function defined on $(0, \infty)$ such that $(-1)^{k+j} F^{(k+j)}(t)$ is nonnegative, nonincreasing, and convex for $j = 0, 1, \ldots, l-2$ on $(0, \infty)$ (if $l = 1$, we require only that it be nonnegative and nonincreasing), it follows that $F(\sqrt{t}) \in \mathscr{P}_k(R^s)$.*

The proof of this theorem uses a result from Askey [4].
Finally, we will prove

Theorem 2.3. *Suppose F' is completely monotonic but not constant on $(0, \infty)$, F is continuous on $[0, \infty)$ and positive on $(0, \infty)$. Then for any distinct vectors $x^1, \ldots, x^n \in R^s$ (s arbitrary)*

$$(-1)^{n-1} \det F(\|x^i - x^j\|^2) > 0.$$

Consequently, the choice $F(t) = (1 + t)^{1/2}$ in Theorem 2.3 proves Franke's conjecture.

Before we prove these theorems we recall the important notion of an almost positive definite matrix, which is relevant to our discussion (see Donoghue [7]).

Definition 2.2. *A real $n \times n$ symmetric matrix A is called almost negative definite provided that*

$$\sum_{j=1}^{n} \sum_{i=1}^{n} c_i c_j A_{ij} \leq 0$$

whenever $\sum_{i=1}^{n} c_i = 0$.

Let us denote this class by $\mathscr{A}$ and note that if $A_{ij} = \|x^i - x^j\|^2$ for some $x^1, \ldots, x^n \in R^s$, then A is in $\mathscr{A}$, because

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \|x^i - x^j\|^2 = -2 \left\| \sum_{i=1}^{n} c_i x^i \right\|^2 \leq 0 \tag{2.5}$$

when $\sum_{i=1}^{n} c_i = 0$. There is a beautiful converse to this observation (see Schoenberg [25] and Blumenthal [6]) that states

Theorem A. *Let A be an $n \times n$ real symmetric matrix with zero diagonal entries. There exist vectors $x^1, \ldots, x^n \in R^s$ for some s such that $A_{ij} = \|x^i - x^j\|^2$ if and only if A is almost negative definite.*

Besides being useful in distance geometry, the notion of almost positive definite matrices is important in probability theory, where it is used to characterize infinitely divisible laws (see Luckas [18]).

Since the matrix $(\|x^i - x^j\|^2)$ appears in the formulation of Definition 2.1, we can express Theorems 2.1–2.3 in terms of almost positive definite matrices, provided we give the condition (2.3) its proper interpretation. For this purpose, we require

Corollary 2.1. *$A \in \mathscr{A}$ if and only if any one of the following conditions holds:*

(a) *There exist $\sigma = (\sigma_1, \ldots, \sigma_n)$ and $x^1, \ldots, x^n \in R^s$ for some s such that $A_{ij} = \sigma_i + \sigma_j + \|x^i - x^j\|^2$.*

(b) *There exist $\sigma = (\sigma_1, \ldots, \sigma_n)$ and a $B = (B_{ij})$, $i, j = 1, \ldots, n$, that is positive definite such that $A_{ij} = \sigma_i + \sigma_j - B_{ij}$.*

(c) $(e^{-\alpha A_{ij}})$ *is positive definite for all* $\alpha > 0$. *Moreover, it is strictly positive definite if and only if*

$$A_{ij} > \tfrac{1}{2}(A_{ii} + A_{jj}), \qquad i \neq j. \tag{2.6}$$

Proof. For the first two claims it suffices to remark that when $A \in \mathscr{A}$, Theorem A says that there exist $x^1, \ldots, x^n$ such that

$$\|x^i - x^j\|^2 = A_{ij} - \tfrac{1}{2}(A_{ii} + A_{jj}).$$

The first part of assertion (c) is a well-known characterization of the class $\mathscr{A}$ (see Donoghue [7]). As for the last claim, when $A \in \mathscr{A}$ inequality (2.6) means that in the representation for A in part (a) the points $x^1, \ldots, x^n \in R^s$ are distinct. Hence we need only recall that $(e^{-\alpha\|x^i - x^j\|^2})$ is strictly positive definite because of the formula

$$e^{-\alpha^2\|x^i - x^j\|^2/2} = (2\pi)^{-s/2} \int_{R^s} e^{i\alpha x \cdot x^i} e^{-i\alpha x \cdot x^j} e^{-\|x\|^2/2}\, dx \tag{2.7}$$

and the linear independence of $e^{ix\cdot x^1}, \ldots, e^{ix\cdot x^n}$, $x \in R^s$ ∎

We will have occasion to use several subclasses of $\mathscr{A}$. First, the distance matrices in $\mathscr{A}$, i.e., matrices with zero diagonal entries, will be denoted by $\mathscr{A}^d$. We let $\mathscr{A}^+$ be the matrices in $\mathscr{A}$ with nonnegative entries and $\mathscr{A}^s$ be the subclass of $\mathscr{A}^+$ for which part (c) of Corollary 2.1 holds.

With these facts at hand, we are now ready to prove Theorems 2.1–2.3.

3. Proofs

We begin with

Lemma 3.1. *If* $\sum_{i=1}^n c_i p(x^i) = 0$ *for all* $p \in \pi_{k-1}(R^s)$ *then*

$$(-1)^k \sum_{i=1}^n \sum_{j=1}^n c_i c_j \|x^i - x^j\|^{2k} \geq 0, \tag{3.1}$$

where equality holds in (3.1) *if and only if*

$$\sum_{i=1}^n c_i p(x^i) = 0, \qquad p \in \pi_k(R^s). \tag{3.2}$$

Remark 3.1. Applying Lemma 3.1 inductively, we see that the conditions

$$\sum_{i=1}^n c_i p(x^i) = 0, \qquad p \in \pi_k(R^s),$$

and

$$\sum_{j=1}^n \sum_{i=1}^n c_i c_j q(\|x^i - x^j\|^2) = 0, \qquad q \in \pi_k(R^1) \tag{3.3}$$

are equivalent. This remark leads us to our final definition.

Definition 3.1. *For any class $\mathscr{M}$ of symmetric matrices with nonnegative entries we let $\mathscr{F}_k(\mathscr{M})$ denote all continuous functions $F(t)$, $t \in [0, \infty)$, such that for any $A \in \mathscr{M}$, $\sum_{i=1}^n \sum_{j=1}^n c_i c_j F(A_{ij}) \geq 0$ whenever*

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j q(A_{ij}) = 0 \qquad \text{for all } q \in \pi_{k-1}(R^1).$$

Remark 3.2. The proofs we present below show also that $F \in \mathscr{F}_k(\mathscr{A}^+)$ whenever both F is continuous on $[0, \infty)$ and $(-1)^k F^{(k)}$ is completely monotonic on $(0, \infty)$. In addition, for functions F satisfying the hypothesis of Theorem 2.3 we have that $(-1)^{n-1}\det F(A_{ij}) > 0$ for any $A \in \mathscr{A}^s$. These statements are useful reformulations of Theorems 2.1 and 2.3, as it is sometimes easier to generate matrices in $\mathscr{A}^s$ directly than to express them as the square of mutual Euclidean distances between vectors.

Let us now prove Lemma 3.1.

Proof. First note that

$$\begin{aligned}
&\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \|x^i - x^j\|^{2k} \\
&\quad = \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \left(\|x^i\|^2 + \|x^j\|^2 - 2(x^i, x^j)\right)^k \\
&\quad = \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \sum_{l=0}^{k} \sum_{t_1 + t_2 = k-l} (-1)^l 2^l \binom{k}{l} \frac{k!}{t_1! t_2!} \|x^i\|^{2t_1} \|x^j\|^{2t_2} (x^i, x^j)^l.
\end{aligned}$$

Using our hypothesis on $(c_1, \ldots, c_n)$ we see that whenever $2t_1 + l < k$ or $2t_2 + l < k$ the corresponding summand above is zero. Since $2t_1 + 2t_2 + 2l = 2k$ we must therefore have $2t_1 + l = 2t_2 + l = k$ for the nonzero summands. Hence

(3.4)

$$\begin{aligned}
&= (-1)^k \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \sum_{\substack{l=0 \\ k-l=\text{even}}}^{k} 2^l \binom{k}{l} \binom{k}{(k-l)/2} \|x^i\|^{k-l} \|x^j\|^{k-l} (x^i, x^j)^l \\
&= (-1)^k \sum_{\substack{l=0 \\ k-l=\text{even}}}^{k} 2^l \binom{k}{l} \binom{k}{(k-l)/2} \\
&\quad \times \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \|x^i\|^{k-l} \|x^j\|^{k-l} \sum_{|\alpha|=l} \binom{l}{\alpha} (x^i)^\alpha (x^j)^\alpha \\
&= (-1)^k \sum_{\substack{l=0 \\ k-l=\text{even}}}^{k} 2^l \binom{k}{l} \binom{k}{(k-l)/2} \sum_{|\alpha|=l} \binom{l}{\alpha} \left| \sum_{i=1}^{n} c_i \|x^i\|^{k-l} (x^i)^\alpha \right|^2,
\end{aligned}$$

which proves the inequality (3.1). Furthermore, when (3.2) holds each summand in (3.4) is zero, because $\|x\|^{k-l} x^\alpha$ is a polynomial of degree $\leq k$, since $|\alpha| = l \leq k$

and $k - l$ is even. Conversely, if the quadratic form (3.1) is zero, then the summands in (3.4) corresponding to $l = k$ give

$$\sum_{i=1}^{n} c_i (x^i)^{\alpha} = 0, \qquad \text{all } |\alpha| = k,$$

so that

$$\sum_{i=1}^{n} c_i q(x^i) = 0$$

for all homogeneous polynomials q of degree k. Thus (3.2) follows and the proof is complete. ■

This lemma states that $F(t) = (-1)^l t^l$ is in $\mathscr{P}_k$ for any $l \leq k$, a special case of Theorem 2.1. Next we prove the general case.

Proof of Theorem 2.1. Suppose $(-1)^k F^{(k)}$ is completely monotonic on $(0, \infty)$. Then by a theorem of Bernstein (see Widder [31]),

$$(3.5) \qquad (-1)^k F^{(k)}(t) = \int_0^{\infty} e^{-t\sigma}\, d\mu(\sigma), \qquad t > 0,$$

where $d\mu(\sigma)$ is a Borel measure on $(0, \infty)$. For $\varepsilon > 0$, we define $F_\varepsilon(t) = F(t + \varepsilon)$, so that using (3.5), we get

$$F_\varepsilon(t) - \sum_{l=0}^{k-1} \frac{F_\varepsilon^{(l)}(0)}{l!} t^l = \int_0^{\infty} \frac{e^{-\varepsilon\sigma}}{\sigma^k} \left\{ e^{-t\sigma} - \sum_{l=0}^{k-1} \frac{(-t\sigma)^l}{l!} \right\} d\mu(\sigma).$$

Setting $t = \|x^i - x^j\|^2$ above, multiplying both sides by $c_i c_j$, and summing over i, j, Lemma 3.1 leads to the equation

$$\sum_{j=1}^{n} \sum_{i=1}^{n} c_i c_j F(\|x^i - x^j\|^2 + \varepsilon) = \int_0^{\infty} e^{-\sigma\varepsilon} \sigma^{-k} \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j e^{-\|x^i - x^j\|^2 \sigma}\, d\mu(\sigma)$$

whenever $\sum_{i=1}^{n} c_i p(x^i) = 0$, $p \in \pi_{k-1}(R^s)$ and $\varepsilon > 0$. Hence letting $\varepsilon \to 0^+$, we conclude $F \in \mathscr{P}_k$ because of Eq. (2.7). ■

Remark 3.3. When $x^1, \ldots, x^n$ are distinct, the measure $d\mu$ in (3.5) has mass other than at the origin; i.e., if $F \notin \pi_k(R^1)$ and $F^{(j)}$, $j = 0, 1, \ldots, k - 1$, are continuous on $[0, \infty)$, then F is *strictly* conditionally positive definite of order k.

A converse of Theorem 2.1 can be obtained from arguments given by Schoenberg [27] for the case $k = 0$. In the general case, we need the representation for an F in $\mathscr{P}_k$ given by Gelfand and Vilenkin [13, Chapter II]. For s sufficiently large, we can successively differentiate this equation, by letting $s \to \infty$ and using the asymptotic properties of Bessel functions of large order. Since this is not our main concern here, we do not elaborate on these details. Instead, we give a short proof, based on Corollary 2.1, of a converse for $k = 1$. Thus suppose $F \in \mathscr{P}_1$; then by part (c) of Corollary 2.1 and Schoenberg's theorem [27] we conclude that $G(t) = e^{\alpha F(t)}$ is completely monotonic for $\alpha > 0$. However, for $l \geq 1$, $G^{(l)}(t) = \alpha F^{(l)}(t) + O(\alpha^2)$, so the desired conclusion follows.

Finally, we observe that the method used above gives also

Corollary 3.1 (a) *If* $A \in \mathscr{A}^+$ *and* F *is completely monotonic, then* $(F(A_{ij}))$ *is positive definite.*

(b) $A \in \mathscr{A}^+$ *if and only if* $A_{ij} \geq 0$ *and* $((1+\lambda A_{ij})^{-1})$ *is positive definite for all* $\lambda > 0$.

Proof. The first statement follows from the Bernstein representation (3.5) (when $k = Q$) and part (c) of Corollary 2.1. Thus we see that $A \in \mathscr{A}$ implies $((1+\lambda A_{ij})^{-1})$ is positive definite, because $(1+\lambda t)^{-1}$ is completely monotonic on $[0, \infty)$ for $\lambda > 0$. Conversely, if $((1+\lambda A_{ij})^{-1})$ is positive definite for all $\lambda > 0$, then by Schur's theorem, so is $([1+(\lambda/n)A_{ij}]^{-n})$ for all n (see Donoghue [7]). Letting $n \to \infty$ we get that $(e^{-\lambda A_{ij}})$ is also positive definite, which by Corollary 2.1, part (c), gives $A \in \mathscr{A}$, thereby completing the proof. ■

Let us also observe that part (a) is best possible in the following sense. Suppose A is a symmetric matrix with nonnegative entries such that $(F(A_{ij}))$ is positive definite for any completely monotonic F. Then $A \in \mathscr{A}$, because we can choose $F(t) = e^{-\lambda t}$. Also, given a continuous F such that $F(A_{ij})$ is positive definite for all $A \in \mathscr{A}$, then F is completely monotonic. This is just Schoenberg's theorem, because our hypothesis implies $F(\|x^i - x^j\|^2)$ is positive definite on any R^s and so F is completely monotonic.

Proof of Theorem 2.2. We base the proof of Theorem 2.2 on Williamson's [32] representation formula for any function F satisfying the hypothesis of the theorem. Namely, we have

$$(-1)^k F^{(k)}(t) = \int_0^\infty (1-\sigma t)_+^{l-1}\, d\mu(\sigma), \qquad t > 0,$$

where, as in (3.5), $d\mu(\sigma)$ is a Borel measure on $(0, \infty)$.

Following the proof of Theorem 2.1, we see that it suffices for the proof of Theorem 2.2 to show that the matrix $((1-\|x^i - x^j\|)_+^{l+k-1})$ is positive definite for $x^1, \ldots, x^n \in R^s$.

Askey [4] pointed out that $((1-\|x^i-x^j\|^\delta)_+)$ is positive definite on R^s when $\delta \geq [s/2]+1$. For the best lower bound of $(s+1)/2$, see (6.9) of Gasper [12] and references therein. ■

Next we prove Theorem 2.3.

Proof of Theorem 2.3. The condition on F and the method of proof used for Theorem 2.1 shows that the matrix $A_{ij} = F(\|x^i - x^j\|^2)$ is in $\mathscr{A}$, and in fact its quadratic form $\sum_{i=1}^n \sum_{j=1}^n c_i c_j A_{ij}$ is zero for $\sum_{i=1}^n c_i = 0$ if and only if $c_i = 0$, $i = 1, \ldots, n$. Since we also have $\sum_{i=1}^n \sum_{j=1}^n A_{ij} > 0$, the theorem follows from the elementary

Lemma 3.2. *Let* A *be a real symmetric* $n \times n$ *matrix such that*

(i) $\sum_{i=1}^n \sum_{j=1}^n c_i c_j A_{ij} \leq 0$ *whenever* $\sum_{i=1}^n c_i = 0$ *with equality if and only if* $c_i = \cdots = c_n = 0$,

(ii) *There is some vector* $d \in R^n$ *such that*

$$\sum_{i=1}^{n} \sum_{j=1}^{n} d_i d_j A_{ij} > 0.$$

Then A has one positive and $n - 1$ *negative eigenvalues.* ■

Generally, if A is negative definite on a subspace of codimension m, for instance when $A_{ij} = -F(\|x^i - x^j\|^2)$, $m = \dim \pi_{k-1}(R^s)$, and $F \in \mathscr{P}_k(R^s)$, then A has at least $n - m$ negative eigenvalues.

Let us now turn to some examples.

4. Examples

Several important examples come from the function $F(t) = 1/(r^2 + t)^\alpha$, $r \geq 0$, $\alpha > 0$. This function is clearly completely monotonic on $(0, \infty)$. Hence the matrix

$$\left((r^2 + \|x^i - x^j\|^2)^{-\alpha}\right) \tag{4.1}$$

is strictly positive definite for all $r > 0$ and $\alpha > 0$. Furthermore, recalling that any time $F(\|x - y\|^2)$ is positive definite we must have $|F(t)| \leq F(0)$, $t > 0$, we see that $\alpha > 0$ is also necessary for (4.1) to be positive definite.

The positive definiteness of $1/(1 + \|x\|^2)^\alpha$ on R^s for $\alpha > s/2$ can also be seen in the following way. The Fourier transform of this function can be computed explicitly:

$$H(x) = \int_{R^s} \frac{e^{ix \cdot y}}{(1 + \|y\|^2)^\alpha} \, dy = \frac{(2\pi)^{s/2}}{\|x\|^{s/2-1}} \int_0^\infty \frac{1}{(1 + \sigma^2)^\alpha} \sigma^{s/2} J_{s/2-1}(\|x\|\sigma) \, d\sigma,$$

which, according to Abramowitz and Stegun [1, p. 488] gives

$$H(x) = \int_{R^s} \frac{e^{ix \cdot y}}{(1 + \|x\|^2)^\alpha} \, dy = \frac{(2\pi)^{s/2}}{2^{\alpha-1} \|x\|^{s/2-\alpha} \Gamma(\alpha)} K_{s/2-\alpha}(\|x\|). \tag{4.2}$$

[K_α is sometimes called Macdonald's function (Watson [30, pp. 78–79]).] Furthermore, $K_\alpha(x) > 0$ for $x > 0$ (see Abramowitz and Stegun [1, p. 374]), which substantiates, by Fourier inversion, the positive definiteness of $(1 + \|x\|^2)^{-\alpha}$, $\alpha > s/2$, $x \in R^s$. We also mention that Macdonald's function gives the reproducing kernel for fractional Sobolev spaces. Specifically, if we let

$$H_\alpha = \left\{ f \in L^2(R^s) \colon \int_{R^s} (1 + \|x\|^2)^\alpha |\hat{f}(x)|^2 \, dx < \infty \right\},$$

where

$$\hat{f}(x) = (2\pi)^{-s} \int_{R^s} e^{-ix \cdot y} f(y) \, dy,$$

then for $\alpha > s/2$ the reproducing kernel of H_α is given by

$$R_\alpha(x) = \int_{R^s} (1 + \|y\|^2)^{-\alpha} e^{ix \cdot y} \, dy,$$

which in view of (4.2) gives

$$R_\alpha(x) = \frac{(2\pi)^{s/2}}{2^{\alpha-1}\|x\|^{s/2-\alpha}\Gamma(\alpha)} K_{s/2-\alpha}(\|x\|). \tag{4.3}$$

Now, let us observe that the kth indefinite integral of F is given by

$$F^{(-k)}(t) = \frac{1}{(1-\alpha)(2-\alpha)\dots(k-\alpha)}(r^2+t)^{k-\alpha}.$$

Thus, choosing $0 < \alpha < 1$, we see that $(r^2+t)^{k-\alpha}$ is strictly k-positive definite. Letting $\alpha \to 0^+$ we get that $-(r^2+t)^k \log(r^2+t)$ is also k-positive definite. These last two examples correspond to the TPS method.

Next we describe the relationship of these functions to Riesz potentials (see Helgason [16, p. 64]).

According to the proof of Theorem 2.1, we have for $0 < \alpha < 1$

$$\frac{(-1)^k}{(1-\alpha)\dots(k-\alpha)} \sum_{i=1}^n \sum_{j=1}^n c_i c_j (1 + \|x^i - x^j\|^2)^{k-\alpha}$$
$$= \int_0^\infty t^{-k} \sum_{i=1}^n \sum_{j=1}^n c_i c_j e^{-t\|x^i - x^j\|^2} \frac{t^{\alpha-1}}{\Gamma(\alpha)} e^{-t}\, dt$$

if $\sum_{i=1}^n c_i p(x^i) = 0$, $p \in \pi_{k-1}(R^s)$. If we scale x^i by $(1/\sqrt{h})x^i$ and let $h \to 0^+$, we get for $k \geq 1$

$$\frac{(-1)^k}{(1-\alpha)\dots(k-\alpha)} \sum_{i=1}^n \sum_{j=1}^n c_i c_j \|x^i - x^j\|^{2(k-\alpha)} \tag{4.4}$$
$$= \frac{1}{\Gamma(\alpha)} \int_0^\infty t^{\alpha-1} \left(\sum_{i=1}^n \sum_{j=1}^n c_i c_j e^{-\|x^i - x^j\|^2 t} \Big/ t^k \right) dt.$$

This formula is independent of the "base" space R^s in which x lies. Alternatively, using Riesz potentials we get for $\alpha > s/2$ and $\alpha = s/2 \notin Z^+$ the identity (4.5)

$$2^{s-2\alpha}\pi^{s/2} \frac{\Gamma(s/2-\alpha)}{\Gamma(\alpha)} \sum_{i=1}^n \sum_{j=1}^n c_i c_j \|x^i - x^j\|^{2\alpha - s} = \int_{R^s} \left(\left| \sum_{k=1}^n c_k e^{i x^k \cdot y} \right|^2 \Big/ \|y\|^{2\alpha} \right) dy$$

when $\sum_{i=1}^n c_i p(x^i) = 0$, $p \in \pi_{k-1}(R^s)$, and $k \geq \alpha - s/2$. Hence, choosing $\alpha = \tau + s/2$, we see that $(-1)^k t^\tau$ is strictly conditionally positive definite of order k for $k - 1 < \tau \leq k$, which already follows from (4.4). When $k = 1$, this result was observed by von Neumann and Schoenberg [22] for $\tau = \frac{1}{2}$. Furthermore, by Corollary 2.1 and the fact that $(\|x^i - x^j\|^{2\tau}) \in \mathscr{A}^d$ for $0 < \tau \leq 1$, we see that $(1 + \|x\|^\tau)^{-\mu}$ is strictly positive definite for $\mu > 0$, $0 < \tau \leq 2$. For the case $s = 1$, $\mu = 1$, see Linnik [17].

Following the advice of Remark 3.2, we are ready to give a stronger version of inequality (1.1). Since $(\|x^i - x^j\|^{2\tau}) \in \mathscr{A}^s$ for $0 < \tau < 1$, we get

$$(-1)^{n-1} \det(r^2 + \|x^i - x^j\|^{2\tau})^\delta > 0$$

whenever $r \geq 0$, $0 < \delta < 1$, $0 < \tau \leq 1$, and $x^1, \ldots, x^n$ are distinct vectors in R^s. Also using Corollary 2.1, we obtain the well-known fact that $e^{-\lambda\|x-y\|^\tau}$, $0 < \tau \leq 2$, is strictly positive definite for any $\lambda > 0$. The function $e^{-\lambda\|x\|^\tau}$ is the characteristic function of a *stable law* (see Luckas [18, p. 36]). For $\tau = 2$, the Gaussian case, this kernel is used in Schagen [24] for scattered data interpolation; they are also discussed by Agterberg [2].

Finally, we remark that the following formula can easily be verified:

$$\frac{(2\pi)^{s/2}}{2^{\alpha-1}\Gamma(\alpha)} \frac{(-1)^{n+1}}{2^n n!} \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \|x^i - x^j\|^{2n} \log \|x^i - x^j\|$$

$$= \int_{R^s} \left(\left| \sum_{l=1}^{n} c_l e^{ix^l \cdot y} \right| \bigg/ \|y\|^{2\alpha} \right) dy$$

when $\sum_{l=1}^{n} c_l p(x^l) = 0$, $p \in \pi_n(R^s)$, $n = \alpha - s/2$. This equation can be compared to

$$\frac{1}{(k-1)!} \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \|x^i - x^j\|^{2(k-1)} \log \|x^i - x^j\|^2$$

$$= \int_0^\infty \left(\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j e^{-t\|x^i - x^j\|^2} \bigg/ (-t)^k \right) dt$$

when $\sum_{i=1}^{n} c_i p(x^i) = 0$, $p \in \pi_{k-1}(R^s)$, $k \geq 1$, which comes from (4.4) by using the expansion $\|x-y\|^{2\alpha} = 1 + 2\alpha \log \|x-y\| + O(\alpha^2)$. Similarly, we have

$$-\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \log\left(1 + \|x^i - x^j\|^2\right)$$

$$= \int_0^\infty \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j e^{-\|x^i - x^j\|^2 t} e^{-t} \frac{dt}{t}$$

if $\sum_{i=1}^{n} c_i = 0$.

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