

Conditionally Positive Definite Functions and Their Application to Multivariate Interpolations

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We derive integral representations for conditionally positive definite functions of various types. Using these representations, we show that certain symmetric linear combinations of translates of conditionally positive definite functions are positive definite functions and can be employed in multivariate scattered data interpolation. We also obtain a necessary and sufficient condition for the smoothness of conditionally positive definite functions. As a corollary, we establish a generalization of a theorem of von Neumann and Schoenberg on integral representation for functions of negative type which play a central role in isometric imbedding theory and radial basis function interpolation. © 1993 Academic Press, Inc.

1. INTRODUCTION

For a natural number m , let $C^m(\mathbb{R}^d)$ denote the class of all complex-valued functions on \mathbb{R}^d which have continuous derivatives up to and including total order m . $C(\mathbb{R}^d)$ will denote the class of all complex-valued continuous functions on \mathbb{R}^d .

In this paper, we use the standard multi-index notations. If $\alpha = (\alpha_1, \dots, \alpha_d)$ and $\beta = (\beta_1, \dots, \beta_d)$ are multi-indices, then (1) $|\alpha| := \sum_{j=1}^d \alpha_j$, (2) $\alpha! := \alpha_1! \cdots \alpha_d!$, (3) $D^\alpha := D_1^{\alpha_1} \cdots D_d^{\alpha_d}$, where $D_j := \partial/\partial x_j$, (4) $\alpha \leq \beta$ means $\alpha_j \leq \beta_j$ for $1 \leq j \leq d$, (5) $\alpha \pm \beta := (\alpha_1 \pm \beta_1, \dots, \alpha_d \pm \beta_d)$. If $x \in \mathbb{R}^d$ and $\xi \in \mathbb{R}^d$, then (6) $x\xi := x_1\xi_1 + \cdots + x_d\xi_d$, (7) $|x| := (x_1^2 + \cdots + x_d^2)^{1/2}$, (8) $x^\alpha := x_1^{\alpha_1} \cdots x_d^{\alpha_d}$.

We note that the absolute value sign in (1) and (7) has different meanings. But this should cause no confusion. In (3), (6), (7), and (8), we used (x_1, \dots, x_d) to denote the coordinates of the point $x \in \mathbb{R}^d$. In what follows, we also use x_1, \dots, x_n to denote a set of n points in \mathbb{R}^d as readers can easily discriminate the meanings from the contexts.

Let k be a nonnegative integer. A function $f \in C(\mathbb{R}^d)$ is said to be

conditionally positive definite of degree k if for any n complex numbers c_1, \dots, c_n , and any n points x_1, \dots, x_n in \mathbb{R}^d satisfying

$$\sum_{j=1}^n c_j x_j^\alpha = 0, \quad |\alpha| < k, \quad (1.1a)$$

we have

$$\sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l f(x_j - x_l) \geq 0. \quad (1.1b)$$

If $k=0$, then the condition in Eq. (1.1a) is vacuous. Thus, a function is conditionally positive definite of degree 0 if and only if it is positive definite. We shall use $CP_k(\mathbb{R}^d)$ to denote the set of all conditionally positive definite functions of degree k on \mathbb{R}^d . It is obvious from the definition that $CP_0(\mathbb{R}^d) \subset CP_1(\mathbb{R}^d) \subset CP_2(\mathbb{R}^d) \subset \dots$.

If f is radial, i.e., there exists a function $h: \mathbb{R}_+ \rightarrow \mathbb{R}$ such that $f(x) = h(|x|)$ for all $x \in \mathbb{R}^d$, and if for all $d = 1, 2, \dots$, we have $-f \in CP_1(\mathbb{R}^d)$, then h is often referred to as a *function of negative type*; see Wells and Williams [WW]. Functions of negative type play a central role in the isometric imbeddings of metric spaces into a Hilbert space. Von Neumann and Schoenberg [NS] established a remarkable characterization theorem for functions of negative type. We refer to [WW] for a modern treatment of the theorem and its application in isometric imbedding theory. Recently, conditionally positive definite functions have found interesting applications in some variational problems and data interpolation; see [MN1, MN2, M, B1, B2] and the references cited there.

For the purpose of multivariate scattered data interpolation, we are particularly interested in a subset of $CP_k(\mathbb{R}^d)$, the set of all strictly conditionally positive definite functions of degree k that we define as follows.

A function $f \in C(\mathbb{R}^d)$ is said to be strictly conditionally positive definite of degree k , if for any n complex numbers c_1, \dots, c_n , not all of them are zero, and any n distinct points x_1, \dots, x_n in \mathbb{R}^d satisfying

$$\sum_{j=1}^n c_j x_j^\alpha = 0, \quad |\alpha| < k, \quad (1.2a)$$

we have

$$\sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l f(x_j - x_l) > 0. \quad (1.2b)$$

We use the symbol $SCP_k(\mathbb{R}^d)$ to denote the set of all strictly

conditionally positive definite functions of degree k on \mathbb{R}^d . Micchelli [M] gave a simple criterion (using the theory of completely monotone functions) which shows that for a given k and for any $d = 1, 2, \dots$, the functions $(-1)^k |x|^\gamma$, $2k - 2 < \gamma < 2k$, and $(-1)^k (1 + |x|^2)^{\gamma/2}$ are elements of $SCP_k(\mathbb{R}^d)$. These functions have been shown to provide elegant multivariate interpolation methods; see the review articles of Dyn [D] and Powell [P].

Madych and Nelson [MN1] established the following variational framework for interpolation using a function of $SCP_k(\mathbb{R}^d)$. Let $h \in SCP_k(\mathbb{R}^d)$ be given; one constructs a subspace C_h of $C(\mathbb{R}^d)$ with a certain semi-inner product $(\cdot, \cdot)_h$ which has null space $\Pi_{k-1}(\mathbb{R}^d)$, where $\Pi_{k-1}(\mathbb{R}^d)$ denotes the space of all the d -variable polynomials of degree $k-1$ or less. If x_1, \dots, x_n are n distinct points in \mathbb{R}^d and d_1, \dots, d_n are some arbitrary data, then there exist a unique $p \in \Pi_{k-1}$ and a unique function $s \in C_h$ of the form $s(x) = \sum_{j=1}^n c_j h(x - x_j)$ such that the function $f_0 := p + s$ interpolates the data d_1, \dots, d_n at the points x_1, \dots, x_n ; i.e., $f_0(x_j) = d_j$, $j = 1, \dots, n$. Furthermore, among all functions $f \in C_h$ that satisfy the interpolation conditions $f(x_j) = d_j$, the semi-norm $\|f\|_h = \sqrt{(f, f)_h}$ is minimized by f_0 .

Buhmann [B1, B2] has systematically studied the topic of interpolation and approximation using some conditionally positive definite functions. Among other things, Buhmann gave a construction scheme for some radial conditionally positive definite functions to perform cardinal interpolation.

In this paper, we study theories and applications of conditionally positive definite functions. In Section 2, we introduce notations and present some preliminary results. In Section 3, we establish integral representations for conditionally positive definite functions of various types. In Section 4, we study the smoothness of conditionally positive definite functions. We obtain a necessary and sufficient condition for a conditionally positive definite function to be in the class $C^m(\mathbb{R}^d)$. Our results indicate that local smoothness of a conditionally positive definite function implies global smoothness of the function. As a corollary of the development, we generalize a theorem of von Neumann and Schoenberg [NS] on integral representation of functions of negative type; see also [WW, p. 38 (Theorem 3.1)]. The final section, Section 5, is devoted to the study of symmetric linear combinations of translates of conditionally positive definite functions. We show that these linear combinations are conditionally positive definite of lower degree or positive definite functions. This interesting fact provides the possibility of having a rich family of functions of simple structure which are capable of performing scattered data interpolation.

2. NOTATIONS AND PRELIMINARIES

Let $f \in L^1(\mathbb{R}^d)$. We use the Fourier transform \hat{f} of f in the following form:

$$\hat{f}(\xi) = \int_{\mathbb{R}^d} e^{-i\xi \cdot x} f(x) dx.$$

Following the notations in [GV], we use the letters \mathcal{S} to denote the space of the Schwartz class of infinitely differentiable and rapidly decreasing functions on \mathbb{R}^d , \mathcal{K} the space of infinitely differentiable functions on \mathbb{R}^d with compact support, and \mathcal{L} the image of \mathcal{K} under the Fourier transform. The functions in \mathcal{L} are fully characterized by the well-known Paley–Wiener Theorem; see [Y, p. 166]. The dual spaces of \mathcal{S} , \mathcal{K} , and \mathcal{L} are denoted by \mathcal{S}' , \mathcal{K}' , and \mathcal{L}' , respectively. For readers who are not familiar with the structures of these spaces, we refer to [GV, Chap. 2].

An element in \mathcal{S} , \mathcal{K} , or \mathcal{L} is called a test function, and an element of \mathcal{S}' , \mathcal{K}' , or \mathcal{L}' a distribution. We use the symbol $\langle T, \phi \rangle$ to denote the action of a distribution T on a test function ϕ with the understanding that they come from the right spaces to justify the action. Let T be a distribution; the Fourier transform \hat{T} of T is defined in a standard way according to the equation $\langle \hat{T}, \phi \rangle = \langle T, \hat{\phi} \rangle$. It is well known that the Fourier transform is one-to-one and continuous from \mathcal{S}' onto \mathcal{S}' , and its inverse is also continuous. Let ϕ be a test function; we define the function ϕ^* by $\phi^*(x) = \overline{\phi(-x)}$, and denote the convolution of ϕ and ϕ^* by $\phi * \phi^*$, that is,

$$\phi * \phi^*(x) := (2\pi)^{-d/2} \int_{\mathbb{R}^d} \phi(\xi) \overline{\phi(\xi - x)} d\xi.$$

Let $p(x) = \sum_{|x|=k} a_x x^x$ be a homogeneous polynomial of degree k . We use $p(D) := \sum_{|x|=k} a_x D^x$ to denote the corresponding homogeneous constant-coefficient differential operator of degree k . The following definition was given in [GV, Chap. 2].

DEFINITION 2.1. Let T be a distribution. T is said to be conditionally positive definite of degree k if for every homogeneous linear constant-coefficient differential operator $p(D)$ and all $\phi \in \mathcal{S}$, we have

$$\langle T, (p(D)\phi) * (p(D)\phi)^* \rangle \geq 0.$$

We remark that with the above definition a conditionally positive definite distribution in \mathcal{S}' is automatically one in \mathcal{K}' . Let $f \in C(\mathbb{R}^d)$. Madych and Nelson [MN2] showed that $f \in CP_k(\mathbb{R}^d)$ if and only if f is

conditionally positive definite of degree k as a distribution in \mathcal{S}' under Definition 2.1.

Conditionally positive definite distributions in \mathcal{X}' were characterized in [GV] (Theorem 3, Chapter 2) as follows.

THEOREM 2.2. *Let $T \in \mathcal{X}'$. In order for T to be conditionally positive definite of degree k it is necessary and sufficient that for each $\phi \in \mathcal{X}$, the following equation hold true:*

$$\begin{aligned} \langle T, \phi \rangle = \langle \hat{T}, \hat{\phi} \rangle &= \int_{\mathbb{R}^d \setminus \{0\}} \left[\hat{\phi}(\xi) - \chi(\xi) \sum_{|\alpha|=0}^{2k-1} \frac{D^\alpha \hat{\phi}(0)}{\alpha!} \xi^\alpha \right] d\mu(\xi) \\ &+ \sum_{|\alpha|=0}^{2k} a_\alpha \frac{D^\alpha \hat{\phi}(0)}{\alpha!}. \end{aligned} \tag{2.1}$$

Here μ is a positive tempered Borel measure on $\mathbb{R}^d \setminus \{0\}$ satisfying

$$\int_{0 < |\xi| \leq 1} |\xi|^{2k} d\mu(\xi) < \infty; \tag{2.2}$$

χ is a function in \mathcal{X} so that the function $\chi - 1$ has a zero of order $2k + 1$ at the origin; $a_\alpha = \langle \hat{f}, \chi_\alpha \rangle$ for $|\alpha| < 2k$, where $\chi_\alpha(\xi) := \chi(\xi)\xi^\alpha$; the numbers a_α , $|\alpha| = 2k$, are such that the matrix $(a_{\alpha+\beta})_{|\alpha|=|\beta|=k}$ is nonnegative definite.

In applications, however, we find the choices of the functions χ in (2.1) inconvenient. Thus it is desirable to give a characterization of all conditionally positive definite distributions in \mathcal{S}' as follows.

THEOREM 2.3. *Let $T \in \mathcal{S}'$. In order for T to be conditionally positive definite of degree k it is necessary and sufficient that for each $\phi \in \mathcal{S}$, the following equation hold true:*

$$\begin{aligned} \langle T, \phi \rangle = \langle \hat{T}, \hat{\phi} \rangle &= \int_{\mathbb{R}^d \setminus \{0\}} \left[\hat{\phi}(\xi) - \kappa(\xi) \sum_{|\alpha|=0}^{2k-1} \frac{D^\alpha \hat{\phi}(0)}{\alpha!} \xi^\alpha \right] d\mu(\xi) \\ &+ \sum_{|\alpha|=0}^{2k} a_\alpha \frac{D^\alpha \hat{\phi}(0)}{\alpha!}. \end{aligned} \tag{2.3}$$

Here κ is an analytic function in \mathcal{S} such that the function $\kappa(\xi) - 1$ has a zero of order $2k + 1$ at the origin; the measure μ and the numbers a_α , $|\alpha| = 0, \dots, 2k$, are as described in Theorem 2.2.

The result of this theorem seems to be standard. However, being not able to find a proof in the literature, we give a full proof here.

Proof. Since K is dense in \mathcal{S} under the topology of \mathcal{S} , for each fixed $\phi \in \mathcal{S}$, we can find a sequence $\{\phi_n\}$ in \mathcal{K} such that $\phi_n \rightarrow \phi$ in \mathcal{S} . Recall that the Fourier transform is a one-to-one continuous operator from \mathcal{S} onto \mathcal{S} . Thus we have $\widehat{\phi}_n \in \mathcal{L}$ and $\widehat{\phi}_n \rightarrow \widehat{\phi}$ in \mathcal{S} . Putting ϕ_n in Eq. (2.1), we get

$$\begin{aligned} \langle T, \phi_n \rangle &= \int_{\mathbb{R}^d \setminus \{0\}} \left[\widehat{\phi}_n(\xi) - \chi(\xi) \sum_{|\alpha|=0}^{2k-1} \frac{D^\alpha \widehat{\phi}_n(0)}{\alpha!} \xi^\alpha \right] d\mu(\xi) \\ &\quad + \sum_{|\alpha|=0}^{2k} a_\alpha \frac{D^\alpha \widehat{\phi}_n(0)}{\alpha!}. \end{aligned} \quad (2.4)$$

Since $T \in \mathcal{S}'$ and since μ is a tempered Borel measure on $\mathbb{R}^d \setminus \{0\}$, we let $n \rightarrow \infty$ in Eq. (2.4) and apply the Dominated Convergence Theorem to get

$$\begin{aligned} \langle T, \phi \rangle &= \langle \widehat{T}, \widehat{\phi} \rangle = \int_{\mathbb{R}^d \setminus \{0\}} \left[\widehat{\phi}(\xi) - \chi(\xi) \sum_{|\alpha|=0}^{2k-1} \frac{D^\alpha \widehat{\phi}(0)}{\alpha!} \xi^\alpha \right] d\mu(\xi) \\ &\quad + \sum_{|\alpha|=0}^{2k} a_\alpha \frac{D^\alpha \widehat{\phi}(0)}{\alpha!}. \end{aligned} \quad (2.5)$$

We have also used the continuity of the differential operator D^α on \mathcal{S} in the above argument. Now we wish to replace the function $\chi \in \mathcal{L}$ by an analytic function $\kappa \in \mathcal{S}$. This goal can be achieved by a similar limit process. Let κ be an analytic function in \mathcal{S} such that the function $\kappa(\xi) - 1$ has a zero of order $2k + 1$ at the origin. Since \mathcal{L} is dense in \mathcal{S} , we can find a sequence $\{\chi_n\}$ in \mathcal{L} such that for each n the function $\chi_n(\xi) - 1$ has a zero of order $2k + 1$ at the origin and $\chi_n \rightarrow \kappa$ in \mathcal{S} . In Eq. (2.5), let $\chi = \chi_n$ and then let $n \rightarrow \infty$, and we get the desired result. ■

We remark that in Theorems 2.2 and 2.3, the measure μ and the numbers a_α , $|\alpha| = 2k$, are uniquely determined by the distribution T , while the functions χ and κ and the numbers a_α , $|\alpha| < 2k$ are not. We refer to [GV, p. 188] for a proof of this fact.

3. INTEGRAL REPRESENTATIONS OF CONDITIONALLY POSITIVE DEFINITE FUNCTIONS

In what follows, a lemma in [GS] (Lemma 2.1) is frequently used. For the convenience of reference, we state the lemma here but do not give a proof.

LEMMA 3.1. Let $x_1, \dots, x_n \in \mathbb{R}^d$ and $c := (c_1, \dots, c_n) \in \mathbb{R}^n$. Assume that

$$\sum_{j=1}^n c_j p(x_j) = 0 \quad \text{for all } p \in \Pi_{k-1}(\mathbb{R}^d).$$

Let $q \in \Pi_m(\mathbb{R}^d)$ and $q_1(x) = \sum_{j=1}^n \sum_{l=1}^n c_j c_l q(x - x_j + x_l)$. Then $q_1 \in \Pi_{m-2k}(\mathbb{R}^d)$. Here if $m - 2k$ is negative, we interpret $\Pi_{m-2k}(\mathbb{R}^d)$ as the set containing only the zero polynomial.

Let $q \in \Pi_{2k-1}(\mathbb{R}^d)$. By Lemma 3.1, we have

$$\sum_{j=1}^n \sum_{l=1}^n c_j c_l q(x_j - x_l) = 0,$$

provided that the points x_1, \dots, x_n and the numbers c_1, \dots, c_n satisfy (1.1a). It follows that $\Pi_{2k-1}(\mathbb{R}^d) \subset CP_k(\mathbb{R}^d)$. However, we also have the following result:

PROPOSITION 3.2. If q is a polynomial of degree m , $m > 2k$, then q is not an element of $CP_k(\mathbb{R}^d)$.

Proof. Let $q(x) = \sum_{|\alpha|=0}^m c_\alpha x^\alpha$ with $c_\alpha \neq 0$ for some $|\alpha| = m$. Let $\phi \in \mathcal{S}$ and $p(D) = \sum_{|\alpha|=k} a_\alpha D^\alpha$ be a homogeneous constant-coefficient differential operator of degree k . Then we have

$$\widehat{p(D)\phi}(\xi) = \sum_{|\alpha|=k} a_\alpha (i\xi)^\alpha \widehat{\phi}(\xi).$$

It is well known that q , as a tempered distribution, has the Fourier transform

$$\widehat{q} = \sum_{|\alpha|=0}^m c_\alpha i^\alpha \delta^{(\alpha)},$$

where δ denotes the Dirac distribution and $\delta^{(\alpha)}$ its distributional derivatives. Hence, we have

$$\begin{aligned} \langle q, (p(D)\phi) * (p(D)\phi)^* \rangle &= \langle \widehat{q}, (\widehat{p(D)\phi})(\widehat{p(D)\phi}) \rangle \\ &= \left\langle \sum_{|\alpha|=0}^m c_\alpha i^\alpha \delta^{(\alpha)}, \left| \sum_{|\alpha|=k} a_\alpha (i\xi)^\alpha \widehat{\phi}(\xi) \right|^2 \right\rangle. \end{aligned} \quad (3.1)$$

Using Eq. (3.1) and the assumption that $c_\alpha \neq 0$ for some $|\alpha| = m > 2k$, we can easily find an analytic function $\phi \in \mathcal{S}$ and a homogeneous constant-coefficient differential operator $p(D)$ of degree k such that $\langle q, (p(D)\phi) * (p(D)\phi)^* \rangle < 0$. Thus, $q \notin CP_k(\mathbb{R}^d)$. ■

LEMMA 3.3. Let $q \in \Pi_{2k}(\mathbb{R}^d)$. Write q in the form $q(x) = q_1(x) + \sum_{|\alpha|=2k} a_\alpha x^\alpha / \alpha!$, where $q_1 \in \Pi_{2k-1}(\mathbb{R}^d)$. Assume that the matrix $(a_{\alpha+\beta})_{|\alpha|=|\beta|=k}$ is nonnegative definite. Then for any n complex numbers c_1, \dots, c_n and any n points $x_1, \dots, x_n \in \mathbb{R}^d$ satisfying

$$\sum_{j=1}^n c_j x_j^\alpha = 0 \quad \text{for all } |\alpha| < k, \tag{3.2}$$

we have

$$(-1)^k \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l q(x_j - x_l) \geq 0. \tag{3.3}$$

If we assume that the matrix $(a_{\alpha+\beta})_{|\alpha|=|\beta|=k}$ is positive definite, then equality in (3.3) holds if and only if $\sum_{j=1}^n c_j x_j^\alpha = 0$ for all $|\alpha| \leq k$.

Remark. If $q(x) = |x|^{2k}$, then the matrix $(a_{\alpha+\beta})_{|\alpha|=|\beta|=k}$ is a diagonal matrix with positive entries on the diagonal line, and therefore is positive definite. Thus, Lemmas 3.1 and 3.3 generalize the results of Lemma 3.1 in [M].

Proof. Let $c_1, \dots, c_n \in \mathbb{C}$ and $x_1, \dots, x_n \in \mathbb{R}^d$ satisfy (3.2). By Lemma 3.1, we have

$$(-1)^k \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l q_1(x_j - x_l) = 0.$$

Hence, we write

$$\begin{aligned} & (-1)^k \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l q(x_j - x_l) \\ &= (-1)^k \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l \sum_{|\alpha|=2k} a_\alpha \frac{(x_j - x_l)^\alpha}{\alpha!} \\ &= (-1)^k \sum_{|\alpha|=2k} \frac{a_\alpha}{\alpha!} \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l \sum_{\beta+\gamma=\alpha} \frac{\alpha!}{\beta! \gamma!} (-1)^{|\beta|} x_j^\beta x_l^\gamma \\ &= (-1)^k \sum_{|\alpha|=2k} a_\alpha \sum_{\beta+\gamma=\alpha} (-1)^{|\beta|} \left(\sum_{j=1}^n c_j \frac{x_j^\beta}{\beta!} \right) \left(\sum_{l=1}^n \bar{c}_l \frac{x_l^\gamma}{\gamma!} \right) \\ &= \sum_{|\alpha|=2k} \sum_{\substack{\beta+\gamma=\alpha \\ |\beta|=|\gamma|=k}} a_{\beta+\gamma} \left(\frac{1}{\beta!} \sum_{j=1}^n c_j x_j^\beta \right) \left(\frac{1}{\gamma!} \sum_{l=1}^n \bar{c}_l x_l^\gamma \right) \\ &= \sum_{|\alpha|=|\beta|=k} a_{\alpha+\beta} A_\alpha \bar{A}_\beta \geq 0, \end{aligned} \tag{3.4}$$

where $A_\beta := (1/\beta!) \sum_{j=1}^n c_j x_j^\beta$. This proves the first part of the lemma. To prove the second part of the lemma, we notice that if there exists an $\alpha, |\alpha| = k$, such that $\sum_{j=1}^n c_j x_j^\alpha \neq 0$, then the positive definiteness of the matrix $(a_{\alpha+\beta})_{|\alpha|=|\beta|=k}$ implies that strict inequality holds in the last step in (3.4). ■

THEOREM 3.4. *Let $f \in C(\mathbb{R}^d)$. In order for f to be an element of $CP_k(\mathbb{R}^d)$, it is necessary and sufficient that f have the following integral representation:*

$$f(x) = \int_{\mathbb{R}^d \setminus \{0\}} [e^{-ix\xi} - \kappa(\xi) T_{2k-1}(e^{-ix\xi})] d\mu(\xi) + \sum_{|\alpha|=0}^{2k} a_\alpha \frac{(-ix)^\alpha}{\alpha!}. \quad (3.5)$$

Here $T_{2k-1}(e^{-ix\xi})$ denotes the $(2k-1)$ th truncated Taylor expansion of the function $\xi \mapsto e^{ix\xi}$ at $\xi = 0$; μ is a positive Borel measure on $\mathbb{R}^d \setminus \{0\}$ satisfying

$$\int_{0 < |\xi| \leq 1} |\xi|^{2k} d\mu(\xi) < \infty \quad \text{and} \quad \int_{|\xi| \geq 1} d\mu(\xi) < \infty;$$

the function κ and the numbers $a_\alpha, |\alpha| \leq 2k$, are as in Theorem 2.3.

Proof. The necessity part can be proved by using Theorem 2.3 and some standard limit arguments; see the first half of the proof of Theorem 1.8 in [GHS] for detail. To prove the sufficiency part, assume that $f \in C(\mathbb{R}^d)$ has been expressed in the form of (3.5). Let $c_1, \dots, c_n \in \mathbb{C}$ and $x_1, \dots, x_n \in \mathbb{R}^d$ be such that $\sum_{j=1}^n c_j x_j^\alpha = 0$ for all $|\alpha| < k$. Let $q_1(x) = \sum_{|\alpha|=0}^{2k-1} (-ix)^\alpha / \alpha!$, and let $q_2(x) = \sum_{|\alpha|=2k} (-ix)^\alpha / \alpha!$. By Lemma 3.1, we have

$$\sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l q_1(x_j - x_l) = 0.$$

By Lemma 3.3, we have

$$\begin{aligned} & \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l q_2(x_j - x_l) \\ &= \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l \sum_{|\alpha|=2k} a_\alpha (-i)^{2k} \frac{(x_j - x_l)^\alpha}{\alpha!} \\ &= (-1)^k \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l \sum_{|\alpha|=2k} a_\alpha \frac{(x_j - x_l)^\alpha}{\alpha!} \geq 0. \end{aligned}$$

Thus, we have

$$\begin{aligned} & \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l f(x_j - x_l) \\ &= \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l q_1(x_j - x_l) + \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l q_2(x_j - x_l) \\ & \quad + \int_{\mathbb{R}^d \setminus \{0\}} \left| \sum_{j=1}^n c_j e^{-ix_j \xi} \right|^2 d\mu(\xi) \geq 0. \quad \blacksquare \end{aligned} \tag{3.6}$$

As a consequence of Theorem 3.4, we characterize the polynomials in the set $\Pi_{2k}(\mathbb{R}^d) \cap CP_k(\mathbb{R}^d)$ as follows.

COROLLARY 3.5. *Let $q \in \Pi_{2k}$. Write q in the form $q(x) = q_1(x) + \sum_{|\alpha|=2k} a_\alpha (x^\alpha / \alpha!)$, where $q_1 \in \Pi_{2k-1}(\mathbb{R}^d)$. Then $(-1)^k q \in CP_k(\mathbb{R}^d)$ if and only if the matrix $(a_{\alpha+\beta})_{|\alpha|=|\beta|=k}$ is nonnegative definite.*

Proof. The sufficiency part follows from Lemma 3.3. The necessity part follows from Theorem 3.4 with the observation that the measure μ and the numbers a_α , $|\alpha| = 2k$, in Equation (3.5) are uniquely determined by the function f . \blacksquare

By imposing a mild condition on the measure μ , we give a sufficient condition for a function f in $CP_k(\mathbb{R}^d)$ to be an element of $SCP_k(\mathbb{R}^d)$.

THEOREM 3.6. *Let $f \in CP_k(\mathbb{R}^d)$ be represented as in (3.5). If the measure μ is not concentrated on a set of Lebesgue measure 0, then $f \in SCP_k(\mathbb{R}^d)$.*

Proof. Let $c_1, \dots, c_n \in \mathbb{C}$ and $x_1, \dots, x_n \in \mathbb{R}^d$ be n distinct points satisfying (1.2a). Then by (3.6), we have

$$\sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l f(x_j - x_l) \geq \int_{\mathbb{R}^d \setminus \{0\}} \left| \sum_{j=1}^n c_j e^{-ix_j \xi} \right|^2 d\mu(\xi) > 0.$$

Here the strict inequality follows from the fact that the function $\sum_{j=1}^n c_j e^{-ix_j \xi}$ is analytic on \mathbb{R}^d and is not identically 0, and therefore can only vanish on a set of Lebesgue measure 0 and the assumption that the measure μ is not concentrated on a set of Lebesgue measure 0. \blacksquare

For radial conditionally positive definite functions, a more compact integral representation was obtained by Guo *et al.* [GHS] (Theorem 1.8).

Let Ω_d denote the Fourier transform of the rotationally invariant probability measure on the unit sphere S_{d-1} of \mathbb{R}^d ; that is,

$$\Omega_d(x) = \omega_{d-1}^{-1} \int_{S_{d-1}} e^{-ix\xi} d\omega,$$

where ω_{d-1} denotes the area of S_{d-1} and $d\omega$ the Lebesgue measure restricted on S_{d-1} . It is obvious that Ω_d is radial and it is well known that the following expansion for Ω_d holds (see [S]),

$$\Omega_d(r) = \sum_{l=0}^{\infty} \frac{(-1)^l r^{2l}}{(2l)!! \prod_{q=0}^{l-1} (d+2q)},$$

where the product $\prod_{q=0}^{l-1} (d+2q)$ is interpreted as 1 if $l=0$.

THEOREM 3.7 [GHS]. *Let f be a radial continuous function on \mathbb{R}^d . In order for f to an element of $CP_k(\mathbb{R}^d)$ it is necessary and sufficient that f have the following integral representation:*

$$f(x) = \int_0^{\infty} \left[\Omega_d(|x|r) - \kappa(r) \sum_{l=0}^{k-1} \frac{(-1)^l r^{2l} |x|^{2l}}{(2l)!! \prod_{q=0}^{l-1} (d+2q)} \right] r^{-2k} d\gamma(r) + \sum_{l=0}^{k-1} \frac{(-1)^l \langle \hat{f}, \kappa(r) r^{2l} \rangle}{(2l)!! \prod_{q=0}^{l-1} (d+2q)} |x|^{2l}, \tag{3.7}$$

where $\kappa(r) = e^{-r^2} \sum_{l=0}^{k-1} r^{2l}/l!$; $\gamma(r)$ is a positive Borel measure on $[0, \infty)$ satisfying $\int_1^{\infty} r^{-2k} d\gamma(r) < \infty$.

Discussion. In the case $k=1$, (3.7) gives integral representation of radial conditionally positive definite functions of degree 1 in the form

$$\int_0^{\infty} [\Omega_d(|x|r) - e^{-r^2}] r^{-2} d\gamma(r) + c, \tag{3.8}$$

where γ is a positive Borel measure on $[0, \infty)$ satisfying $\int_1^{\infty} r^{-2} d\gamma(r) < \infty$, and c is a constant.

The classical result of von Neumann and Schoenberg [NS] asserts that any such function with $f(0) = 0$ can be represented as

$$\int_0^{\infty} [\Omega_d(|x|r) - 1] r^{-2} d\gamma(r), \tag{3.9}$$

where γ is a positive Borel measure on $[0, \infty)$ satisfying $\int_1^{\infty} r^{-2} d\gamma(r) < \infty$.

To see that these two integral representations are essentially the same, we write

$$\begin{aligned} & \int_0^\infty [\Omega_d(|x| r) - e^{-r^2}] r^{-2} d\gamma(r) \\ &= \int_0^\infty [\Omega_d(|x| r) - 1 + 1 - e^{-r^2}] r^{-2} d\gamma(r) \\ &= \int_0^\infty [\Omega_d(|x| r) - 1] r^{-2} dy(r) + c_1, \end{aligned}$$

where $c_1 := \int_0^\infty [1 - e^{-r^2}] r^{-2} d\gamma(r)$ is a constant. The split of the integrals in the above calculation is justified by the property of the function Ω_d and the measure γ . The above discussion consists of a special case of the general development in Section 4 in which we study the relationships between the smoothness of a conditionally positive functions and the growth condition of the measure μ in the integral representation.

Using Theorem 3.7, we can characterize those radial functions that are in $SCP_k(\mathbb{R}^d)$.

THEOREM 3.8. *In order for a radial function f to be an element of $SCP_k(\mathbb{R}^d)$, $d \geq 2$, it is necessary and sufficient that f have the integral representation (3.7) and that the measure $\gamma(r)$ is not concentrated at the point $r = 0$.*

Proof. To prove the necessity, assume that the measure γ is concentrated at $r = 0$. In this case, Eq. (3.7) shows $f(x) = A |x|^{2k}$, where A is a constant. Let $c_1, \dots, c_n \in \mathbb{C}$ and $x_1, \dots, x_n \in \mathbb{R}^d$ be n distinct points such that $\sum_{j=1}^n |c_j| > 0$ and $\sum_{j=1}^n c_j x_j^\alpha = 0$ for all $|\alpha| \leq k$. Then these c_j 's and x_j 's satisfy (1.2a). However, by Lemma 3.1, we have

$$\sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l f(x_j - x_l) = 0.$$

Therefore, f is not an element of $SCP_k(\mathbb{R}^d)$.

To prove the sufficiency, let $c_1, \dots, c_n \in \mathbb{C}$ and $x_1, \dots, x_n \in \mathbb{R}^d$ be n distinct points such that $\sum_{j=1}^n |c_j| > 0$ and $\sum_{j=1}^n c_j x_j^\alpha = 0$ for all $|\alpha| < k$. Recall the fact that in \mathbb{R}^d , $d \geq 2$, the n functions $e^{-ix_j \cdot \xi}$, $j = 1, 2, \dots, n$, are linearly independent on the sphere $|x| = r$, $r > 0$. Thus for any $r > 0$, we have

$$\sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l \Omega_d(|x_j - x_l|) = \omega_{d-1}^{-1} \int_{S_{d-1}} \left| \sum_{j=1}^n c_j e^{-ix_j \cdot r\omega} \right|^2 d\omega > 0.$$

By Lemma 3.1 and the assumption that the measure γ is not concentrated on the point $r=0$, we have

$$\sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l f(x_j - x_l) = \int_0^\infty \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l \Omega_d(|x_j - x_l| r) r^{-2k} d\gamma(r) > 0.$$

This shows that $f \in SCP_k(\mathbb{R}^d)$. ■

The following problem is both practically important and theoretically interesting. For a fixed k , characterize those continuous functions $h: \mathbb{R}_+ \rightarrow \mathbb{R}$ for which the functions $H(x) := h(|x|^2)$ are elements of $CP_k(\mathbb{R}^d)$ for all $d = 1, 2, \dots$

The cases $k=0, 1$ were settled by Schoenberg [S]. Micchelli [M] studied the general case and gave a sufficient condition. A complete solution was recently given by Guo *et al.* [GHS] as in the following theorem.

THEOREM 3.9. *Let $h \in C([0, \infty))$, and let $H(x) := h(|x|^2)$. In order that the function H be an element of $CP_k(\mathbb{R}^d)$, it is necessary and sufficient that the function $g(t) := h(t^2)$ have the integral representation*

$$g(t) = \int_0^\infty \left[e^{-t^2 r^2} - \kappa(r) \sum_{l=0}^{k-1} (-1)^l \frac{t^{2l} r^{2l}}{l!} \right] r^{-2} d\beta(r) + \sum_{l=0}^{k-1} a_l t^{2l}, \quad (3.10)$$

where a_l are some constants, $\kappa(r) = e^{-r^2} \sum_{l=0}^{k-1} r^{2l}/l!$, and $\beta(r)$ is a positive Borel measure on $[0, \infty)$ such that $\int_1^\infty r^{-2k} d\beta(r) < \infty$. Here the summation $\sum_{l=0}^{k-1}$ is interpreted as 0 if $k=0$.

Remarks. (i) In (3.10), the measure β is uniquely determined by the function h . The function $\kappa(r)$ can be replaced by any other analytic function $\theta(r)$ on $[0, \infty)$ the satisfies (a) $1 - \theta(r)$ has a zero of order $2k$ at the $r=0$; (b) θ is rapidly decreasing in the sense that $\lim_{r \rightarrow 0} \theta(r) p(r) = 0$ for any fixed polynomial $p(r)$; (c) the numbers $a_l, l=0, \dots, k-1$, depend on the function κ .

(ii) Recall that a function $h \in C([0, \infty))$ is said to be completely monotone if $(-1)^l h^{(l)}(t) \geq 0$ for each $l=0, 1, 2, \dots$, and all $t \in (0, \infty)$. It is elementary to see that Eq. (3.10) holding true for the function $g, g(t) := h(t^2)$, is equivalent to the function $(-1)^k h^{(k)}$ being completely monotone on $(0, \infty)$.

(iii) In the case $k=1$, Eq. (3.10) gives

$$g(t) = \int_0^\infty (e^{-t^2 r^2} - e^{-r^2}) r^{-2} d\beta(r) + c, \quad (3.11)$$

where c is a constant. Equation (3.11) can be re-written in the form

$$g(t) = \int_0^\infty (e^{-t^2 r^2} - 1) r^{-2} d\beta(r) + c_1,$$

where c_1 is a constant. This conforms with the integral representation given by Schoenberg [S, Theorem 6].

We have three equivalent conditions for a function to be in the set $\bigcap_{d=1}^\infty SCP_k(\mathbb{R}^d)$.

THEOREM 3.10. *Let $h \in C([0, \infty))$. The following three statements are equivalent:*

- (i) *The function $H(x) := h(|x|^2) \in \bigcap_{d=1}^\infty SCP_k(\mathbb{R}^d)$.*
- (ii) *The function $g(t)$ can be represented as in Eq. (3.10), where the measure β is not concentrated at the point $r=0$.*
- (iii) *$(-1)^k h^{(k)}$ is completely monotone on $(0, \infty)$ and $h^{(k)}$ is not a constant.*

Proof. (i) \Rightarrow (ii). Assume that $H \in \bigcap_{d=1}^\infty SCP_k(\mathbb{R}^d)$. We only need to show that the measure $\beta(r)$ is not concentrated at $r=0$. Suppose that it is. Then Eq. (3.10) shows that the function g is a polynomial of degree at most $2k$. Therefore H is not an element of $\bigcap_{k=1}^\infty SCP_k(\mathbb{R}^d)$ for any d .

(ii) \Rightarrow (iii). Assume that (ii) is true. For $t > 0$, we can successively differentiate under the integral sign to see that the function $(-1)^k h^{(k)}$ is completely monotone on $(0, \infty)$. To show that $h^{(k)}$ is not a constant, assume the contrary. Then the function g is a polynomial of degree at most $2k$. Since the measure β is uniquely determined by the function g , β must be concentrated at $r=0$. This is a contradiction.

(iii) \Rightarrow (i) was proved by Micchelli [M, Theorem 2.1]. \blacksquare

4. THE SMOOTHNESS OF CONDITIONALLY POSITIVE DEFINITE FUNCTIONS

Except for being continuous, functions in $CP_k(\mathbb{R}^d)$ may not have any other smoothness property. In fact, there are positive definite functions which are nowhere differentiable; see Schoenberg [S]. In this section, we obtain a necessary and sufficient condition for the smoothness of functions in $CP_k(\mathbb{R}^d)$ based on the theory of Gelfand and Vilenkin [GV] on conditionally positive definite distributions and the integral representations given in the last section. As a corollary of the development, we establish a generalization of the theorem of von Neumann and Schoenberg [NS].

Let Δ denote the Laplacian operator. Δ^m is iteratively defined by $\Delta^m = \Delta(\Delta^{m-1})$ with $\Delta^1 = \Delta$.

THEOREM 4.1. *Let $f \in CP_k(\mathbb{R}^d)$ and let l be a nonnegative integer. Then the following three statements are equivalent:*

- (i) $\Delta^l f$ is continuous in some neighborhood of the origin.
- (ii) The measure μ in the integral representation of f as in Eq. (3.5) satisfies the additional condition $\int_{|\xi| \geq 1} |\xi|^{2l} d\mu(\xi) < \infty$.
- (iii) f belongs to $C^{2l}(\mathbb{R}^d)$.

Proof. We only need to prove the implications (i) \Rightarrow (ii) and (ii) \Rightarrow (iii). To prove (i) \Rightarrow (ii), assume that (i) is true. We look at f as an element of S' and apply Δ^l to it. We have

$$\langle \Delta^l f, \phi \rangle = \langle f, \Delta^l \phi \rangle = \langle \widehat{f}, \widehat{\Delta^l \phi} \rangle = (-1)^l \langle \widehat{f}, \psi \rangle,$$

where $\psi(\xi) = |\xi|^{2l} \widehat{\phi}(\xi)$.

By Theorem 2.3, we have

$$\begin{aligned} \langle \Delta^l f, \phi \rangle &= (-1)^l \int_{\mathbb{R}^d \setminus \{0\}} \left[|\xi|^{2l} \widehat{\phi}(\xi) - \chi(\xi) \sum_{|\alpha|=0}^{2k-1} \frac{D^\alpha \psi(0)}{\alpha!} \xi^\alpha \right] d\mu(\xi) \\ &\quad + \sum_{|\alpha|=0}^{2k} a_\alpha \frac{D^\alpha \psi(0)}{\alpha!}. \end{aligned} \tag{4.1}$$

Let θ be a infinitely differentiable and compactly supported function such that $\int_{\mathbb{R}^d} \theta(x) dx = 1$. For $\varepsilon > 0$, let θ_ε be the function defined by $\theta_\varepsilon = (1/\varepsilon^d) \theta(\varepsilon^{-1}x)$. In Eq. (4.1), let $\phi = \theta_\varepsilon$, and then let $\varepsilon \downarrow 0$. By the assumption on f , we have $\langle \Delta^l f, \theta_\varepsilon \rangle \rightarrow \Delta^l f(0)$. Denote the function $\xi \mapsto |\xi|^{2l} \widehat{\theta}_\varepsilon(\xi)$ by Θ_ε . Using the properties of the function χ and the measure μ , it is easy to show that the three functions of ε , $I_1(\varepsilon)$, $I_2(\varepsilon)$, $I_3(\varepsilon)$, are bounded, where

$$\begin{aligned} I_1(\varepsilon) &= \int_{0 < |\xi| \leq 1} \left[|\xi|^{2l} \widehat{\theta}_\varepsilon(\xi) - \chi(\xi) \sum_{|\alpha|=0}^{2k-1} \frac{D^\alpha \Theta_\varepsilon(0)}{\alpha!} \xi^\alpha \right] d\mu(\xi), \\ I_2(\varepsilon) &= \int_{|\xi| \geq 1} \left[\chi(\xi) \sum_{|\alpha|=0}^{2k-1} \frac{D^\alpha \Theta_\varepsilon(0)}{\alpha!} \xi^\alpha \right] d\mu(\xi), \\ I_3(\varepsilon) &= \sum_{|\alpha|=0}^{2k} a_\alpha \frac{D^\alpha \Theta_\varepsilon(0)}{\alpha!}. \end{aligned}$$

This forces $\int_{|\xi| \geq 1} |\xi|^{2l} \widehat{\theta}_\varepsilon(\xi) d\mu(\xi)$ to be bounded. Since $\widehat{\theta}_\varepsilon(\xi)$ converges to 1 uniformly on any compact set of \mathbb{R}^d , it follows that $\int_{|\xi| \geq 1} |\xi|^{2l} d\mu(\xi) < \infty$. This proves the implication (i) \Rightarrow (ii).

To prove (ii) \Rightarrow (iii), assume $\int_{|\xi| \geq 1} |\xi|^{2l} d\mu(\xi) < \infty$. Under this condition, for $|\alpha| \leq 2l$, and each $x \in \mathbb{R}^d$, the function

$$\xi \mapsto D_x^\alpha [e^{-ix\xi} - \chi(\xi) T_{2k-1}(e^{-ix\xi})]$$

is continuous on \mathbb{R}^d and absolutely integrable with respect to the measure μ on $\mathbb{R}^d \setminus \{0\}$. By invoking Theorem 3.4, we can differentiate under the integral sign of Eq. (3.5) and apply the Lebesgue Dominated Convergence Theorem to get

$$D_x^\alpha f(x) = \int_{\mathbb{R}^d \setminus \{0\}} D_x^\alpha [e^{-ix\xi} - \chi(\xi) T_{2k-1}(e^{-ix\xi})] d\mu(\xi) + D_x^\alpha \left(\sum_{|\alpha|=0}^{2k} a_\alpha \frac{(-ix)^\alpha}{\alpha!} \right).$$

We see that $D_x^\alpha f$ is continuous everywhere in an obvious way. \blacksquare

What is interesting in Theorem 4.1 is that local smoothness of a conditionally positive definite function implies global smoothness of the function.

If f belongs to the set $CP_k(\mathbb{R}^d) \cap C^{2k}(\mathbb{R}^d)$, then we can express f in a better form, as the following theorem shows.

THEOREM 4.2. *Let $f \in CP_k(\mathbb{R}^d)$. Assume that $f \in C^{2k}(\mathbb{R}^d)$. Then we have*

$$f(x) = \int_{\mathbb{R}^d \setminus \{0\}} [e^{-ix\xi} - T_{2k-1}(e^{-ix\xi})] d\mu(\xi) + \sum_{|\alpha|=0}^{2k-1} \frac{(D^\alpha f)(0)}{\alpha!} + (-1)^k \sum_{|\alpha|=2k} a_\alpha \frac{x^\alpha}{\alpha!},$$

where μ is a positive Borel measure on $\mathbb{R}^d \setminus \{0\}$ satisfying $\int_{\mathbb{R}^d \setminus \{0\}} |\xi|^{2k} d\mu(\xi) < \infty$, and the numbers a_α , $|\alpha| = 2k$, are such that the matrix $(a_{\alpha+\beta})_{|\alpha|=|\beta|=k}$ is nonnegative definite.

Proof. In Eq. (3.5), replace the function χ by χ_ε , where $\chi_\varepsilon(\xi) := \chi(\varepsilon\xi)$, $\varepsilon > 0$; then let $\varepsilon \downarrow 0$. Since $\chi_\varepsilon(\xi)$ converges to 1 uniformly on any compact set of \mathbb{R}^d and the measure μ satisfies $\int_{\mathbb{R}^d \setminus \{0\}} |\xi|^{2k} d\mu(\xi) < \infty$, by the Dominated Convergence Theorem, for each $x \in \mathbb{R}^d$, the integral

$$\int_{\mathbb{R}^d \setminus \{0\}} [e^{-ix\xi} - \chi_\varepsilon(\xi) T_{2k-1}(e^{-ix\xi})] d\mu(\xi)$$

converges to the integral

$$\int_{\mathbb{R}^d \setminus \{0\}} [e^{-ix\xi} - T_{2k-1}(e^{-ix\xi})] d\mu(\xi).$$

It is clear that when $\varepsilon \downarrow 0$, $\hat{\chi}_\varepsilon$ converges to the distribution δ in \mathcal{S}' . Denote the function $\xi \mapsto \chi_\varepsilon(\xi) \xi^\alpha$ by Φ_ε . For $|\alpha| < 2k$, we have

$$a_\alpha = \langle \hat{f}, \Phi_\varepsilon \rangle = \langle f, \widehat{\Phi}_\varepsilon \rangle = (-i)^{|\alpha|} \langle f, D^\alpha \widehat{\chi}_\varepsilon \rangle = i^{|\alpha|} \langle D^\alpha f, \widehat{\chi}_\varepsilon \rangle.$$

Therefore, a_α converges to $i^{|\alpha|} D^\alpha f(0)$, and $(-i)^{|\alpha|} a$ to $D^\alpha f(0)$, $|\alpha| < 2k$. Theorem 4.2 is thus proved. ■

We recall that in the proof of Theorem 3.7 [GHS, Theorem 1.8], the measure γ was constructed by letting $\gamma(r) = \int_{0 < |\xi| \leq r} |\xi|^{2k} d\mu(p)$. Hence, for $l \leq k$, $\int_{|\xi| \geq 1} |\xi|^{2l} d\mu(\xi) < \infty$ if and only if $\int_1^\infty r^{-2(k-l)} d\gamma(r) < \infty$. The following theorem then follows naturally.

THEOREM 4.3. *Let $f \in CP_k(\mathbb{R}^d)$. Assume that f is radial. Then the following three statements are equivalent:*

- (i) $\Delta^l f$ is continuous in some neighborhood of the origin.
- (ii) The measure γ in the integral representation of f as in Eq. (3.7) satisfies $\int_1^\infty r^{-2(k-l)} d\gamma(r) < \infty$.
- (iii) f belongs to $C^{2l}(\mathbb{R}^d)$.

Using Theorem 3.7 and a similar argument in the proof of Theorem 4.2, we obtain the following elegant representation for radial functions belonging to the set $CP_k(\mathbb{R}^d) \cap C^{2(k-1)}(\mathbb{R}^d)$.

THEOREM 4.4. *Let $k \geq 1$ and $f \in CP_k(\mathbb{R}^d)$. Assume that f is radial and that $\Delta^{k-1} f$ belongs to $C(\mathbb{R}^d)$. Then the following representation for f holds true,*

$$f(x) = \int_0^\infty \left[\Omega_d(|x|r) - \sum_{i=0}^{k-1} \frac{(-1)^i r^{2i} |x|^{2i}}{(2i)!! \prod_{q=0}^{i-1} (d+2q)} \right] r^{-2k} d\gamma(r) + \sum_{i=0}^{k-1} \frac{\Delta^i f(0)}{(2i)!! \prod_{q=0}^{i-1} (d+2q)} |x|^{2i},$$

where γ is a positive Borel measure on $[0, \infty)$ satisfying $\int_1^\infty r^{-2} dr < \infty$.

Note that in Theorem 4.4, we only assumed that $\Delta^{k-1} f$ is continuous. This is possible because of the fact that the polynomial in Eq. (3.7) has no odd terms. Theorem 4.4 yields the following simple consequence.

COROLLARY 4.5. *Let f be a radial function. Then f belongs to the class $CP_1(\mathbb{R}^d)$ if and only if f has the integral representation*

$$f(x) = \int_0^\infty \frac{\Omega_d(|x| r) - 1}{r^2} d\gamma(r) + f(0), \tag{4.2}$$

where γ is a positive Borel measure on $[0, \infty)$ satisfying $\int_1^\infty r^{-2} d\gamma(r) < \infty$.

Stated in the language of isometric imbedding, von Neumann and Schoenberg's theorem [NV] (see also [WW, Theorem 9.1]) is equivalent to Corollary 4.5.

5. LINEAR COMBINATIONS OF TRANSLATES
OF CONDITIONALLY POSITIVE DEFINITE FUNCTIONS

A remarkable property of functions in $CP_k(\mathbb{R}^d)$ is that the degree of the conditionally positive definiteness can be reduced by forming symmetric linear combinations of their translates.

THEOREM 5.1. *Let $f \in CP_k(\mathbb{R}^d)$. Let $d_1, \dots, d_m \in \mathbb{C}$ and $y_1, \dots, y_m \in \mathbb{R}^d$ be such that $\sum_{s=1}^m d_s y_s^\alpha = 0$ for all $|\alpha| < k_1 \leq k$. Set $g(x) := \sum_{s=1}^m \sum_{t=1}^m d_s \bar{d}_t f(x - y_s - y_t)$. Then $g \in CP_{k-k_1}(\mathbb{R}^d)$.*

Proof. We first show that if $\sum_{j=1}^n c_j x_j^\alpha = 0$ for all $|\alpha| < k - k_1$, and if $\sum_{s=1}^m d_s y_s^\alpha = 0$ for all $|\alpha| < k_1$, then

$$\sum_{j=1}^n \sum_{s=1}^m c_j d_s (x_j - y_s)^\alpha = 0 \quad \text{for all } |\alpha| < \alpha. \tag{5.1}$$

In fact, we have

$$\begin{aligned} & \sum_{j=1}^n \sum_{s=1}^m c_j d_s (x_j - y_s)^\alpha \\ &= \sum_{\beta \leq \alpha} (-1)^{|\beta|} \frac{\alpha!}{\beta! (\alpha - \beta)!} \sum_{j=1}^n \sum_{s=1}^m c_j d_s x_j^{\alpha - \beta} y_s^\beta \\ &= \sum_{\beta \leq \alpha} (-1)^{|\beta|} \frac{\alpha!}{\beta! (\alpha - \beta)!} \left[\sum_{j=1}^n c_j x_j^{\alpha - \beta} \right] \left[\sum_{s=1}^m d_s y_s^\beta \right]. \end{aligned} \tag{5.2}$$

If $|\alpha| < k$, then either $|\alpha - \beta| < k - k_1$ or $|\beta| < k_1$. Therefore (5.2) implies that (5.1) is true.

Now we verify that $g \in CP_{k-k_1}(\mathbb{R}^d)$. Let $c_1, \dots, c_n \in \mathbb{C}$ and $x_1, \dots, x_n \in \mathbb{R}^d$ be such that $\sum_{j=1}^n c_j x_j^\alpha = 0$ for all $|\alpha| < k - k_1$. We have

$$\begin{aligned} & \sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l g(x_j - x_l) \\ &= \sum_{j=1}^n \sum_{l=1}^n \sum_{s=1}^m \sum_{t=1}^m c_j \bar{c}_l d_s \bar{d}_t f((x_j - x_l) - (y_s - y_t)) \\ &= \sum_I \sum_J C_I \bar{C}_J f(X_I - X_J), \end{aligned}$$

where $C_I = c_j d_s$, $X_I = x_j - y_s$, and the summation indices I, J run over a set of cardinality mn . By (5.1), we have $\sum_I C_I X_I^\alpha = 0$ for all $|\alpha| < k$. Since $f \in CP_k(\mathbb{R}^d)$, (5.3) shows that

$$\sum_{j=1}^n \sum_{l=1}^n c_j \bar{c}_l g(x_j - x_l) \geq 0.$$

This shows that $g \in CP_k(\mathbb{R}^d)$. ■

The converse of Theorem 5.1 is also true. Namely, if a function $f \in C(\mathbb{R}^d)$ has the property that for any $d_1, \dots, d_m \in \mathbb{C}$ and $y_1, \dots, y_m \in \mathbb{R}^d$ satisfying $\sum_{s=1}^m d_s y_s^\alpha = 0$ for all $|\alpha| < k_1 \leq k$, we have $g(x) := \sum_{s=1}^m d_s \sum_{t=1}^m \bar{d}_t f(x - y_s + y_t) \in CP_{k-k_1}(\mathbb{R}^d)$, then $f \in CP_k(\mathbb{R}^d)$. In fact, using a limit argument, we show that the following is true: if $\phi \in \mathcal{S}$ satisfies

$$\int_{\mathbb{R}^d} \phi(x) x^\alpha dx = 0, \quad |\alpha| < k_1,$$

and if $\psi \in \mathcal{S}$ satisfies

$$\int_{\mathbb{R}^d} \psi(x) x^\alpha dx = 0, \quad |\alpha| < k - k_1,$$

then

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} f(w - x + y - z) \phi(w) \overline{\phi(x)} \psi(y) \overline{\psi(z)} dw dx dy dz \geq 0. \quad (5.4)$$

Equation (5.4) shows that

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} f(x - y) \Phi(x) \overline{\Phi(y)} dx dy \geq 0,$$

where $\Phi = \phi * \psi$. Since the set of such functions Φ is dense in the set

$\{\phi : \int_{\mathbb{R}^d} \phi(x) x^\alpha dx = 0, |\alpha| < k\}$, by Lemma 1.3 and Theorem 6.1 in [MN2], we have $f \in CP_k(\mathbb{R}^d)$.

THEOREM 5.2. *Let $f \in CP_k(\mathbb{R}^d)$. Assume that the measure μ in the integral representation of (3.5) is not concentrated on a set of Lebesgue measure 0. Let $d_1, \dots, d_m \in \mathbb{C}$ and $y_1, \dots, y_m \in \mathbb{R}^d$ be n distinct points satisfying*

$$\sum_{s=1}^m d_s y_s^\alpha = 0 \quad \text{for all } |\alpha| < k_1 \leq k, \quad \text{and} \quad \sum_{s=1}^m |d_s| > 0.$$

Set $g(x) := \sum_{s=1}^m \sum_{t=1}^m d_s \bar{d}_t f(x - y_s - y_t)$. Then $g \in SCP_{k-k_1}(\mathbb{R}^d)$.

Proof. We first express f in its integral form as in (3.5). Denote the polynomial part of the right hand side of (3.5) by q . Since $q \in CP_k(\mathbb{R}^d)$, by Theorem 5.1, we have

$$\sum_{s=1}^m \sum_{t=1}^m d_s \bar{d}_t q(x - y_s - y_t) \in CP_{k-k_1}(\mathbb{R}^d).$$

Therefore, to prove Theorem 5.2, it suffices to show that

$$\sum_{s=1}^m \sum_{t=1}^m d_s \bar{d}_t f_1(x - y_s - y_t) \in SCP_{k-k_1}(\mathbb{R}^d),$$

where f_1 denotes the integral part of the right hand side of (3.5). Let $c_1, \dots, c_n \in \mathbb{C}$ and let x_1, \dots, x_n be n distinct points in \mathbb{R}^d satisfying

$$\sum_{j=1}^n c_j y_j^\alpha = 0 \quad \text{for all } |\alpha| < k - k_1, \quad \text{and} \quad \sum_{j=1}^n |c_j| > 0.$$

By Lemma 3.1, we have

$$\begin{aligned} & \sum_{j=1}^n \sum_{t=1}^m c_j \bar{c}_t \sum_{s=1}^m \sum_{l=1}^m d_s \bar{d}_l f(x_j - x_l + y_s - y_t) \\ &= \int_{\mathbb{R}^d \setminus \{0\}} \left| \sum_{s=1}^m d_s e^{-iy_s \xi} \right|^2 \left| \sum_{j=1}^n c_j e^{-ix_j \xi} \right|^2 d\mu(\xi) > 0. \end{aligned}$$

The last inequality is true because the measure μ is not concentrated on a set of Lebesgue measure 0. ■

The corresponding result for radial conditionally positive definite functions appears more elegant as in the following theorem.

THEOREM 5.3. *Let f be a radial function in $SCP_k(\mathbb{R}^d)$. Let $d_1, \dots, d_m \in \mathbb{C}$ and $y_1, \dots, y_m \in \mathbb{R}^d$ be n distinct points satisfying*

$$\sum_{s=1}^m d_s y_s^\alpha = 0 \quad \text{for all } |\alpha| < k_1 \leq k, \quad \text{and} \quad \sum_{s=1}^m |d_s| > 0.$$

Set $g(x) := \sum_{s=1}^m \sum_{t=1}^m d_s \bar{d}_t f(x - y_s - y_t)$. Then $g \in SCP_{k-k_1}(\mathbb{R}^d)$.

We omit the proof of Theorem 5.3, since it follows from Theorem 3.7 with a slight modification of the proof of Theorem 5.2.

In particular, Theorems 5.2 and 5.3 show that certain symmetric linear combinations of conditionally positive definite functions can be strictly positive definite, and therefore can be applied to scattered data interpolation. Some special cases of this result have been studied in [GS]. The following interesting phenomenon has been observed by many authors: while some useful conditionally positive definite functions do not decay at infinity, a certain symmetric linear combination of their translates does at a desirable rate. Therefore, in implementing these interpolation schemes, we can estimate both the lower and the upper bounds of the interpolation matrices in terms of the dimension d and the minimum separation distance of the data points. It is also possible to extend the interpolation scheme to “infinite scattered interpolation,” which includes “cardinal interpolation” (interpolation on the integer lattice of \mathbb{R}^d) as a special case. The details of this investigation will appear in a forthcoming paper.

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