On Unbounded Positive Definite Functions

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Abstract

It is well known that positive definite functions are bounded, taking their maximum absolute value at 0. Nevertheless, there are unbounded functions, arising e.g. in potential theory or the study of (continuous) extremal measures, which still exhibit the general characteristics of positive definiteness. Taking a framework set up by Lionel Cooper as a motivation, we study the general properties of such functions which are positive definite in an extended sense. We prove a Bochner-type theorem and, as a consequence, show how unbounded positive definite functions arise as limits of classical positive definite functions, as well as that their space is closed under convolution. Moreover, we provide criteria for a function to be positive definite in the extended sense, showing in particular that complete monotonicity in conjunction with absolute integrability is sufficient.

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1. Introduction

The concept of positive definite sequences, arising naturally in the context of a problem in complex function theory posed by Carathéodory [5], was introduced in 1911 by Toeplitz [22]. Herglotz [8] established a connection between positive definite sequences and the trigonometric moment problem. Motivated by the work of Carathéodory and Toeplitz, Mathias [12] and later Bochner [3] defined and studied the properties of positive definite functions, specifically their harmonic analysis. Before these developments, however, Mercer [13] had studied the more general concept of positive definite kernels in research on integral equations.

According to the classical standard definition, a function $f : \mathbb{R} \to \mathbb{C}$ is *positive definite* if

$$\sum_{i,j=1}^{n} f(x_i - x_j)\, v_i\, \overline{v_j} \geq 0 \tag{1}$$

for all $x_1, x_2, \dots, x_n \in \mathbb{R}$ and $v_1, v_2, \dots, v_n \in \mathbb{C}$, with any $n \in \mathbb{N}$; in other words, if the matrix $\left[f(x_i - x_j)\right]_{i,j=1}^{n}$ is non-negative definite for all $n \in \mathbb{N}$ and

$x_1, x_2, \ldots, x_n \in \mathbb{R}$. We shall denote the set of classical positive definite functions on $\mathbb{R}$ by $\mathrm{P_C}$. Using (1) with $n = 2$, $x_1 = 0$, $x_2 = x$, $v_1 = 1$ and v_2 such that $v_2 f(x) = -|f(x)|$, it can be shown that $|f(x)| \leq f(0)$ for all $x \in \mathbb{R}$. Hence positive definite functions by the standard definition are always bounded.

However, a positive definite function in this sense need not be positive or continuous; for example, the function $f(x) = 1$ if $x = 0$, $f(x) = 0$ otherwise ($x \in \mathbb{R}$), is positive definite, but not continuous; the cosine function is positive definite, but not non-negative. For continuous classically positive definite functions, (1) is equivalent to

$$\int_{\mathbb{R}} \int_{\mathbb{R}} f(x-y)\phi(x)\overline{\phi(y)}\, dxdy \geq 0 \tag{2}$$

for all functions $\phi \in \mathrm{C}_0(\mathbb{R})$, see e.g. [6, p.53].

One of the central results on this subject is Bochner's theorem [3, Chapter IV.20], which states that a function $f : \mathbb{R} \to \mathbb{C}$ is continuous and positive definite if and only if it is the (inverse) Fourier transform of a finite, non-negative measure μ on $\mathbb{R}$, i.e.

$$f(x) = \check{\mu}(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{ix\xi}\, \mu(d\xi) \qquad (x \in \mathbb{R}). \tag{3}$$

Thus, Bochner's theorem provides an equivalent characterisation of whether or not a given continuous function f is positive definite. The concept of positive definite functions was extended to positive definite distributions by L. Schwartz [19, Chapter VII, §9], and his analogue of Bochner's theorem states that a distribution is positive definite (and tempered) if and only if it is the Fourier transform of a non-negative measure of slow increase, i.e. such that the measure of balls is polynomially bounded in terms of the radius.

As shown above, positive definite functions in the sense of the standard definition (1) are always bounded by their value at 0. However, there exist functions such as $f = |\cdot|^{-\alpha}$ $(0 < \alpha < 1)$, which are unbounded at the origin, yet still exhibit properties similar to those of positive definite functions. Such functions arise naturally in potential theory (see, e.g. [2], [10] and [14]), and recently appeared in the context of extremal measures ([16], [17]). Functions which are unbounded at the origin and positive definite in the following extended sense were studied by Cooper [6].

Definition 1. A function $f : \mathbb{R} \to \mathbb{C}$ is called *positive definite w.r.t. a set* J of functions if for every $\phi \in J$, the integral in (2) exists (in the Lebesgue sense) and is non-negative [6, p. 54].

Let $\mathrm{P}(J)$ denote the class of all functions which are positive definite w.r.t. the set J. For certain spaces of functions J, Cooper's definition enables us to extend the concept of positive definiteness to functions which have a singularity at 0. In particular, we shall consider the spaces $J = \mathrm{L}^p(\mathbb{R})$ (and their local versions) for various values of p.

Building on the foundations set by Cooper, we study unbounded positive definite functions in more detail. Our central result is Theorem 2, which, in analogy to Bochner's theorem for the classical case, characterises a larger class of (generally unbounded) positive definite functions. Several subsequent results follow from this Theorem. For example, functions which are positive definite w.r.t. $\mathrm{L}^2(\mathbb{R})$ can be approximated, in the $\mathrm{L}^1(\mathbb{R})$ sense, by a sequence of continuous, classically positive definite functions (see Corollary 1). Functions which arise as 'convolution squares' are positive definite in the new sense (see Corollary 4), and conversely, a function which is positive definite w.r.t. $\mathrm{L}^2(\mathbb{R})$ can be written, in some sense, as a convolution square (see Corollary 5). Using Theorem 2, we also show that the even reflections of integrable, completely monotone functions are positive definite w.r.t. $\mathrm{L}^2(\mathbb{R})$ (see Corollary 8). This result provides many examples of functions which have a singularity at zero and are positive definite in the extended sense.

The structure of the paper is as follows. In section 2 we introduce the ideas and discuss the main results of [6]. In section 3 we prove Theorem 2. Sections 4 and 5 present corollaries to Theorem 2 and their proofs. We conclude the paper with several examples of unbounded positive definite functions.

2. Positive definiteness in the extended sense

We begin with an overview of some basic properties of the positive definite functions studied in [6], analogous to those for the classical case, see [21, p. 412]. In the following, let J be a set of complex-valued measurable functions defined on $\mathbb{R}$. This includes functions defined on a non-empty, measurable subset of $\mathbb{R}$, which we consider to be extended by zero to the whole real line. Then the following properties follow directly from Definition 1.

i. $f \in \mathrm{P}(J) \Leftrightarrow f^* \in \mathrm{P}(J)$, where $f^*(x) := \overline{f(-x)}$ $(x \in \mathbb{R})$.

ii. $f \in \mathrm{P}(J) \Leftrightarrow \overline{f} \in \mathrm{P}(J)$ if J is closed under complex conjugation.

iii. If $f_1, f_2, \ldots, f_n \in \mathrm{P}(J)$ and $c_i \geq 0$ $(i = 1, \ldots, n)$, then $\sum_{i=1}^n c_i f_i \in \mathrm{P}(J)$.

Before proceeding to present our new results, we highlight the most relevant results of [6].

For $p \in [1, \infty) \cup \{\infty\}$, let $\mathrm{L}_0^p(\mathbb{R})$ denote the subspace of functions in $\mathrm{L}^p(\mathbb{R})$ with compact essential support. The functions in $\mathrm{P}(\mathrm{L}_0^1(\mathbb{R}))$ are essentially bounded [6, Th. 5] and almost everywhere equal to a continuous, positive definite function in the classical sense [7, Sec. 6]. The functions in $\mathrm{P}(\mathrm{L}_0^2(\mathbb{R}))$ need only be locally integrable [6, Lemma 1]. Cooper has the following Bochner-type theorem [6, Th. 6].

Theorem 1. *For any function $f \in \mathrm{P}(\mathrm{L}_0^2(\mathbb{R}))$, there exists a non-negative, non-decreasing function ρ, such that for almost all x,*

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{ixt} \, d\rho(t) \qquad \textit{in } (\mathrm{C},\ 1) \textit{ sense}, \tag{4}$$

where $\rho(t) = o\,(t)$ as $t \to \pm\infty$.

Note also that, unlike Bochner's theorem, the implication here is only in one direction. The qualification "in (C, 1) sense" in (4) means

$$f(x) = \frac{1}{\sqrt{2\pi}} \lim_{\lambda\to\infty} \frac{1}{\lambda} \int_0^{\lambda} \left(\int_{-u}^{u} e^{ivx}\, d\rho(v) \right) du,$$

in analogy to Cesàro summation of divergent series.

The $\mathrm{P}(\mathrm{L}_0^p(\mathbb{R}))$ spaces have the following additional properties.

Proposition 1. *If $f \in \mathrm{P_C}$ is continuous, then $f \in \mathrm{P}(\mathrm{L}_0^2(\mathbb{R}))$.*

Proof. By Bochner's theorem, there exists a finite, non-negative measure μ on $\mathbb{R}$ such that for any $\phi \in \mathrm{L}_0^2(\mathbb{R})$,

$$\begin{aligned} \int_{\mathbb{R}} \int_{\mathbb{R}} f(x-y)\phi(x)\overline{\phi(y)}\, dxdy &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} e^{i(x-y)\xi}\, \mu(d\xi)\, \phi(x)\overline{\phi(y)}\, dxdy \\ &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \left| \int_{\mathbb{R}} e^{ix\xi}\phi(x)\, dx \right|^2 \mu(d\xi) \geq 0. \end{aligned}$$

□

Proposition 2. *If $f \in \mathrm{P}(\mathrm{L}_0^2(\mathbb{R}))$ and $g \in \mathrm{P_C}$ is continuous, then $fg \in \mathrm{P}(\mathrm{L}_0^2(\mathbb{R}))$* [6, Th. 1].

Proof. By Bochner's theorem, there exists a finite, non-negative measure μ on $\mathbb{R}$ such that for any $\phi \in \mathrm{L}_0^2(\mathbb{R})$,

$$\begin{aligned} &\int_{\mathbb{R}} \int_{\mathbb{R}} fg\,(x-y)\phi(x)\overline{\phi(y)}\, dxdy \\ &\qquad = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \int_{\mathbb{R}} f(x-y) \int_{\mathbb{R}} e^{i(x-y)\xi}\, \mu(d\xi)\, \phi(x)\overline{\phi(y)}\, dxdy \\ &\qquad = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}}\int_{\mathbb{R}}\int_{\mathbb{R}} f(x-y)(e^{ix\xi}\phi(x))(\overline{e^{iy\xi}\phi(y)})\, dxdy\, \mu(d\xi) \geq 0. \end{aligned}$$

□

Proposition 3. *For any $p \in [1, 2]$, $\mathrm{P}(\mathrm{L}_0^p(\mathbb{R})) \subseteq \mathrm{P}(\mathrm{L}_0^2(\mathbb{R}))$.*

Proof. This follows directly from the fact that $\mathrm{L}_0^2(\mathbb{R}) \subseteq \mathrm{L}_0^p(\mathbb{R})$ ($p \in [1, 2]$). □

Proposition 4. *For any $q \in [2, \infty]$ and $r \in [0, \infty]$, $\mathrm{P}(\mathrm{L}_0^2(\mathbb{R})) = \mathrm{P}(\mathrm{L}_0^q(\mathbb{R})) = \mathrm{P}(\mathrm{C}_0^r(\mathbb{R}))$.*

Proposition 4 can be proved using [6, Lemma 1] and the density of $\mathrm{C}_0^\infty(\mathbb{R})$ in $\mathrm{L}_0^q(\mathbb{R})$ ($q \in [2, \infty]$). The proof is similar to that of Lemma 2 below.

The last two propositions demonstrate that as p increases from 1 to 2, $\mathrm{P}(\mathrm{L}_0^p(\mathbb{R}))$ increases from a smaller class of positive definite functions to a larger such class. As p increases beyond 2, $\mathrm{P}(\mathrm{L}_0^p(\mathbb{R}))$ remains the same. Moreover, roughly speaking, as p increases from 1 to 2, $\mathrm{P}(\mathrm{L}_0^p(\mathbb{R}))$ runs from the class of bounded, continuous positive definite functions (in the standard sense), to a class of functions which are positive definite in a wider sense and need not be bounded or continuous.

3. An extension of Bochner's theorem to unbounded positive definite functions

We use Cooper's definition of positive definiteness with $J = \mathrm{L}^2(\mathbb{R})$. For $\mathrm{L}^2(\mathbb{R})$, as opposed to the space of compactly supported functions $\mathrm{L}^2_0(\mathbb{R})$ of Theorem 1, we obtain the following Bochner-type theorem.

Theorem 2. *Let $f \in \mathrm{L}^1(\mathbb{R})$. Then*

$$f \in \mathrm{P}(\mathrm{L}^2(\mathbb{R})) \textit{ if and only if } \hat{f} \geq 0,$$

where $\hat{f}$ denotes the Fourier transform of f.

We remark that under the hypothesis of Theorem 2, f will correspond to a regular, in particular tempered, distribution, and hence Schwartz's version of Bochner's theorem applies. Nevertheless, with regard to applications where both f and its Fourier transform are functions, the above generalised form of Bochner's theorem in Cooper's framework seems of interest, along with its more elementary proof and the further consequences shown in Sections 4 and 5 below. The proof of Theorem 2 will be based upon the following two lemmas.

Lemma 1. *Let $f \in \mathrm{L}^1(\mathbb{R})$ and $\phi \in \mathrm{L}^2(\mathbb{R})$. Then the integral in* (2) *exists, and*

$$\int_{\mathbb{R}} \int_{\mathbb{R}} f(x-y)\phi(x)\overline{\phi(y)}\, dxdy = \int_{\mathbb{R}} f(z)(\phi * \phi^*)(z)\, dz, \tag{5}$$

where $\phi^*(z) = \overline{\phi(-z)}$ $(z \in \mathbb{R})$.

Proof. Since the convolution of two elements of $\mathrm{L}^2(\mathbb{R})$ is in $\mathrm{L}^\infty(\mathbb{R})$,

$$\begin{aligned}\left|\int_{\mathbb{R}} \int_{\mathbb{R}} f(x-y)\phi(x)\overline{\phi(y)}\, dxdy\right| &= \left|\int_{\mathbb{R}} f(z) \int_{\mathbb{R}} \phi(x)\overline{\phi(x-z)}\, dxdz\right| \\ &= \left|\int_{\mathbb{R}} f(z)(\phi * \phi^*)(z)\, dz\right| \leq \|f\|_1 \, \|\phi * \phi^*\|_\infty.\end{aligned}$$

□

Lemma 2. *Let $f \in \mathrm{L}^1(\mathbb{R})$. Then $f \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ if and only if $f \in \mathrm{P}(\mathcal{S}(\mathbb{R}))$, where $\mathcal{S}(\mathbb{R})$ denotes the Schwartz space of rapidly decreasing functions on $\mathbb{R}$.*

Proof. Since $\mathcal{S}(\mathbb{R}) \subset \mathrm{L}^2(\mathbb{R})$, it follows directly that $\mathrm{P}(\mathrm{L}^2(\mathbb{R})) \subset \mathrm{P}(\mathcal{S}(\mathbb{R}))$. For the reverse implication, we shall use the density of $\mathcal{S}(\mathbb{R})$ in $\mathrm{L}^2(\mathbb{R})$. Suppose that $f \in \mathrm{P}(\mathcal{S}(\mathbb{R}))$. Then the integral

$$\int_{\mathbb{R}} \int_{\mathbb{R}} f(x-y)\psi(x)\overline{\psi(y)}\, dxdy = \int_{\mathbb{R}} (f * \psi)\, \overline{\psi} \tag{6}$$

exists in the Lebesgue sense and is non-negative for all $\psi \in \mathcal{S}(\mathbb{R})$. Since $f \in \mathrm{L}^1(\mathbb{R})$ and the convolution of an element of $\mathrm{L}^1(\mathbb{R})$ with an element of $\mathrm{L}^2(\mathbb{R})$ is in $\mathrm{L}^2(\mathbb{R})$, the integral also exists for all $\psi \in \mathrm{L}^2(\mathbb{R})$. By a change of variables and the Fubini theorem,

$$\int_{\mathbb{R}}\int_{\mathbb{R}} f(x-y)\psi(x)\overline{\psi(y)}\,dxdy = \int_{\mathbb{R}}\int_{\mathbb{R}} f(z)\psi(z+y)\overline{\psi(y)}\,dydz \qquad (\psi \in \mathrm{L}^2(\mathbb{R})).$$

Let $\phi \in \mathrm{L}^2(\mathbb{R})$; then there is a sequence $(\psi_n)_{n\in\mathbb{N}}$ in $\mathcal{S}(\mathbb{R})$ such that $\|\phi-\psi_n\|_2 \to 0$ as $n \to \infty$. Now,

$$\begin{aligned}
&\sup_{z\in\mathbb{R}}\left|\int_{\mathbb{R}}\left(\phi(z+y)\overline{\phi(y)} - \psi_n(z+y)\overline{\psi_n(y)}\right)dy\right| \\
&\quad\le \sup_{z\in\mathbb{R}}\int_{\mathbb{R}} |\phi(z+y)||(\phi-\psi_n)(y)|\,dy + \sup_{z\in\mathbb{R}}\int_{\mathbb{R}} |(\phi-\psi_n)(z+y)||\psi_n(y)|\,dy \\
&\quad\le \|\phi\|_2\,\|\phi-\psi_n\|_2 + \|\phi-\psi_n\|_2\,\|\psi_n\|_2 \;\to 0 \quad \text{as } n\to\infty.
\end{aligned}$$

As $f \in \mathrm{L}^1(\mathbb{R})$, it follows that

$$\left|\int_{\mathbb{R}} f(z)\int_{\mathbb{R}}\left(\phi(z+y)\overline{\phi(y)} - \psi_n(z+y)\overline{\psi_n(y)}\right)\,dydz\right| \to 0 \quad \text{as } n\to\infty,$$

and hence

$$\int_{\mathbb{R}}\int_{\mathbb{R}} f(x-y)\phi(x)\overline{\phi(y)}\,dxdy = \lim_{n\to\infty}\int_{\mathbb{R}}\int_{\mathbb{R}} f(x-y)\psi_n(x)\overline{\psi_n(y)}\,dxdy \;\ge 0.$$

□

Proof of Theorem 2. Since $f \in \mathrm{L}^1(\mathbb{R})$, the integral in (6) exists for all $\psi \in \mathcal{S}(\mathbb{R})$. Since the space of Schwartz functions is closed under convolution [20, Th. 3.3], $\psi * \psi^* \in \mathcal{S}(\mathbb{R})$ for all $\psi \in \mathcal{S}(\mathbb{R})$, where $\psi^*(z) = \overline{\psi(-z)}$ $(z \in \mathbb{R})$. Hence, for any $z \in \mathbb{R}$ and $\psi \in \mathcal{S}(\mathbb{R})$,

$$\begin{aligned}
(\psi * \psi^*)\,(z) &= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} (\,\psi * \psi^*\check{)}(x)\,e^{-ixz}\,dx = \int_{\mathbb{R}} \check{\psi}(x)\,\check{\psi^*}(x)\,e^{-ixz}\,dx \\
&= \int_{\mathbb{R}} |\check{\psi}(x)|^2\,e^{-ixz}\,dx,
\end{aligned}$$

since

$$\check{\psi^*}(x) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \overline{\psi(-\xi)}\,e^{i\xi x}\,d\xi = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \overline{\psi(\xi)}\,e^{-i\xi x}\,d\xi = \overline{\check{\psi}}(x) \qquad (x \in \mathbb{R}). \tag{7}$$

By Lemma 1,

$$\begin{aligned}
\int_{\mathbb{R}}\int_{\mathbb{R}} f(x-y)\psi(x)\overline{\psi(y)}\,dxdy &= \int_{\mathbb{R}} f(z)(\psi * \psi^*)(z)\,dz \\
&= \int_{\mathbb{R}}\int_{\mathbb{R}} f(z)\,|\check{\psi}(x)|^2\,e^{-ixz}dxdz = \sqrt{2\pi}\int_{\mathbb{R}} \hat{f}(x)\,|\check{\psi}(x)|^2 dx. \qquad (8)
\end{aligned}$$

From (8) it is clear that if $\hat{f} \geq 0$, then $f \in \mathrm{P}(\mathcal{S}(\mathbb{R}))$. By Lemma 2 it follows that $f \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$.

Conversely, suppose that $\hat{f}(z) < 0$ at some point $z \in \mathbb{R}$. $\hat{f}$ is continuous and bounded because $f \in \mathrm{L}^1(\mathbb{R})$. It follows that $\hat{f}$ is negative on some interval $\mathcal{I} = [z-\delta, z+\delta]$ with $\delta > 0$. Let

$$\psi_1(x) = \begin{cases} \exp\left[\left((x-z)^2 - \delta^2\right)^{-1}\right] & \text{if} \quad z-\delta < x < z+\delta \\ 0 & \text{otherwise} \end{cases} \qquad (x \in \mathbb{R}).$$

Then $\psi_1 \in \mathrm{C}_0^\infty(\mathbb{R}) \subset \mathcal{S}(\mathbb{R})$. For $\psi_2 := \hat{\psi}_1 \in \mathcal{S}(\mathbb{R})$, it follows by (8) that

$$\begin{aligned} 0 &\leq \int_{\mathbb{R}}\int_{\mathbb{R}} f(x-y)\psi_2(x)\overline{\psi_2(y)}\,dxdy = \sqrt{2\pi}\int_{\mathbb{R}} \hat{f}(x)\,|\check{\psi}_2(x)|^2\,dx \\ &= \sqrt{2\pi}\int_{z-\delta}^{z+\delta} \hat{f}(x)\,|\psi_1(x)|^2\,dx < 0, \end{aligned}$$

which is a contradiction. □

Remark. It follows from Theorem 2 that if $f \in \mathrm{L}^1(\mathbb{R}) \cap \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$, then $f = f^*$ almost everywhere. Indeed, $\hat{f^*} = \hat{f} \geq 0$ by (7), and thus $f = f^*$ almost everywhere by the uniqueness of the Fourier transform on $\mathrm{L}^1(\mathbb{R})$ [4, Th. 5].

4. Approximation by positive definite functions and convolution squares

In this section we present some corollaries to Theorem 2. In particular, we show that functions in $\mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ can be approximated by continuous, classically positive definite functions. We also establish connections between functions which are positive definite for $\mathrm{L}^2(\mathbb{R})$ and functions which arise as convolution squares. We begin by proving the following technical lemma, which shows that $\mathrm{L}^1(\mathbb{R}) \cap \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ is a closed subset of $\mathrm{L}^1(\mathbb{R})$.

Lemma 3. *Let $(f_n)_{n\in\mathbb{N}}$ be a sequence of functions such that $f_n \in \mathrm{L}^1(\mathbb{R})$ and $f_n \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ $(n \in \mathbb{N})$. If $\lim_{n\to\infty} \|f_n - f\|_1 = 0$ for some $f \in \mathrm{L}^1(\mathbb{R})$, then $f \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$.*

Proof. Let $\phi \in \mathrm{L}^2(\mathbb{R})$. By Lemma 1,

$$\left|\int_{\mathbb{R}}\int_{\mathbb{R}} (f_n(x-y) - f(x-y))\,\phi(x)\overline{\phi(y)}\,dxdy\right| \leq \|f_n - f\|_1\|\phi * \phi^*\|_\infty \to 0$$

$(n \to \infty)$. Thus,

$$\int_{\mathbb{R}}\int_{\mathbb{R}} f(x-y)\phi(x)\overline{\phi(y)}\,dxdy = \lim_{n\to\infty}\int_{\mathbb{R}}\int_{\mathbb{R}} f_n(x-y)\phi(x)\overline{\phi(y)}\,dxdy \geq 0.$$

□

Lemma 3 is analogous to the pointwise convergence property for the classical positive definite functions, see [21, p. 412].

We now present some consequences of Theorem 2. The first observation is that $\mathrm{L}^1(\mathbb{R}) \cap \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ is the closure of $\mathrm{L}^1(\mathbb{R}) \cap \mathrm{P}_\mathrm{C}$.

Corollary 1. *Let $f \in \mathrm{L}^1(\mathbb{R})$. Then, $f \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ if and only if there is a sequence $(g_n)_{n\in\mathbb{N}}$ of continuous, classically positive definite functions such that $g_n \in \mathrm{L}^1(\mathbb{R})$ $(n \in \mathbb{N})$ and $\lim_{n\to\infty} \|g_n - f\|_1 = 0$.*

Proof. Suppose $f \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$. As $f \in \mathrm{L}^1(\mathbb{R})$, its Fourier transform $\hat{f}$ is continuous, bounded and tends to 0 at $\pm\infty$. Also, by Theorem 2, $\hat{f} \geq 0$. For $n \in \mathbb{N}$, let

$$\eta_n(\xi) = \frac{n}{\sqrt{2\pi}}\, e^{-(n\xi)^2/2} \qquad (\xi \in \mathbb{R}),$$

so that $\int_\mathbb{R} \eta_n(x)\, dx = 1$. Define

$$h_n(\xi) := \sqrt{2\pi}\, \hat{f}(\xi)\, \hat{\eta}_n(\xi) = \hat{f}(\xi)\, e^{-\xi^2/(2n^2)} \geq 0 \qquad (\xi \in \mathbb{R}).$$

Then $h_n \in \mathrm{L}^1(\mathbb{R})$. Let $g_n = \check{h}_n$ be the inverse Fourier transform of h_n. By Bochner's theorem [3, Chapter IV.20], g_n is continuous and classically positive definite. In particular, it has the property that $|g_n(u)| \leq g_n(0) < \infty$ $(u \in \mathbb{R})$. Also, $g_n = f * \eta_n$, so by Young's inequality, $g_n \in \mathrm{L}^1(\mathbb{R})$ $(n \in \mathbb{N})$. Since $f \in \mathrm{L}^1(\mathbb{R})$, it follows that $\lim_{n\to\infty} \|g_n - f\|_1 = 0$ [20, Th. 1.18].

For the reverse direction, we need only show that $g_n \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ $(n \in \mathbb{N})$. Since $g_n \in \mathrm{L}^1(\mathbb{R})$ $(n \in \mathbb{N})$, g_n has a continuous Fourier transform, and it follows from Bochner's theorem that $\hat{g}_n \geq 0$ $(n \in \mathbb{N})$. Thus, $g_n \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ $(n \in \mathbb{N})$ by Theorem 2. □

We show next that $\mathrm{L}^1(\mathbb{R}) \cap \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ is closed under convolution and, under the further assumption of square integrability, under pointwise multiplication as well.

Corollary 2. *Let $f, g \in \mathrm{L}^1(\mathbb{R})$. If $f, g \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ then $f * g \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$.*

Proof. Suppose $f, g \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$. By Theorem 2, $\hat{f}$, $\hat{g} \geq 0$. By Young's inequality, $f * g \in \mathrm{L}^1(\mathbb{R})$; moreover

$$\widehat{f * g} = \sqrt{2\pi}\; \hat{f}\, \hat{g} \geq 0,$$

so $f * g \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ by Theorem 2. □

Corollary 3. *Let $f, g \in \mathrm{L}^1(\mathbb{R}) \cap \mathrm{L}^2(\mathbb{R})$. If $f, g \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ then $fg \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$.*

Proof. Suppose $f, g \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$. By Theorem 2, $\hat{f}$, $\hat{g} \geq 0$. By the Cauchy-Schwarz inequality, $fg \in \mathrm{L}^1(\mathbb{R})$; furthermore

$$\widehat{fg} = \frac{1}{\sqrt{2\pi}}\; \hat{f} * \hat{g} \geq 0,$$

hence $fg \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ by Theorem 2. □

The next statement shows that functions which arise as 'convolution squares' are positive definite in the new sense, note that $p^*(z) = \overline{p(-z)}$ $(z \in \mathbb{R})$ as before.

Corollary 4. *If $f = p * p^*$ for some $p \in \mathrm{L}^1(\mathbb{R})$, then $f \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$.*

Proof. Suppose $f = p * p^*$ with $p \in \mathrm{L}^1(\mathbb{R})$. By Young's inequality, $f \in \mathrm{L}^1(\mathbb{R})$. From (7) it follows that

$$\hat{f} = \widehat{p * p^*} = \sqrt{2\pi}\, \hat{p}\, \hat{p^*} = |\hat{p}|^2 \geq 0.$$

Thus, $f \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ by Theorem 2. $\square$

This result is analogous to the classical result that if $f = g * g^*$ for some $g \in \mathrm{L}^2(\mathbb{R})$, then f is positive definite in the original sense [11, Th. 4.2.4]. Note that in the classical case we have $f \in \mathrm{L}^\infty(\mathbb{R})$, since the convolution of two elements of $\mathrm{L}^2(\mathbb{R})$ is in $\mathrm{L}^\infty(\mathbb{R})$, whereas in our present situation we have $f = p * p^* \in \mathrm{L}^1(\mathbb{R})$, again by Young's inequality.

In Corollary 5 we show that a version of the converse to Corollary 4 is also true, *viz.* that a function which is positive definite w.r.t. $\mathrm{L}^2(\mathbb{R})$ can be written, in some sense, as a convolution square. An analogous statement is known for continuous, classically positive definite functions (Khinchine's criterion, [11, Th. 4.2.5]). In particular, *if $f : \mathbb{R} \to \mathbb{C}$ is a characteristic function then there exists a sequence $(g_n)_{n\in\mathbb{N}}$ of complex-valued functions, such that for any $n \in \mathbb{N}$, $\int_{\mathbb{R}} |g_n(x)|^2\, dx = 1$, and $f(t) = \lim_{n\to\infty} g_n * g_n^*(t)$ holds uniformly in every finite t-interval.* Note that a function $f : \mathbb{R} \to \mathbb{C}$ is a characteristic function if and only if it is continuous, classically positive definite and $f(0) = 1$. The final condition can always be achieved via normalisation due to the bounded nature of classical positive definite functions.

Corollary 5. *Let $f \in \mathrm{L}^1(\mathbb{R})$. If $f \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$, then there is a sequence $(p_n)_{n\in\mathbb{N}}$ of functions such that $p_n \in \mathrm{L}^2(\mathbb{R})$, $p_n * p_n^* \in \mathrm{L}^1(\mathbb{R})$ $(n \in \mathbb{N})$, and $\lim_{n\to\infty} \|p_n * p_n^* - f\|_1 = 0$.*

Proof. Let $g_n = \check{h}_n$ $(n \in \mathbb{N})$ be the functions constructed in the proof of Corollary 1, then $\lim_{n\to\infty} \|g_n - f\|_1 = 0$. By [11, Th. 4.2.4], there exists $p_n \in \mathrm{L}^2(\mathbb{R})$ such that $g_n = p_n * p_n^*$ $(n \in \mathbb{N})$. $\square$

Note that here $p_n \notin \mathrm{L}^1(\mathbb{R})$ in general; also we don't have $\int_{\mathbb{R}} |p_n(x)|^2\, dx = 1$ as in Theorem 4.2.4 (ii) [11], since we do not assume that h_n is the density of a probability measure.

5. Sufficient criteria for generalised positive definiteness

The criterion of Theorem 2 for a function to be positive definite for $\mathrm{L}^2(\mathbb{R})$ is that its Fourier transform is non-negative. We now give sufficient conditions for this.

For a measurable set $I \subset \mathbb{R}$ and $p \in [1, \infty)$, let

$$\mathrm{L}^p(I) = \left\{ f : I \to \mathbb{C} \;\middle|\; \int_I |f(x)|\, dx < \infty \right\}.$$

Naturally $\mathrm{L}^p(I) \subset \mathrm{L}^p(\mathbb{R})$, extending functions by zero on $\mathbb{R} \backslash I$. We always use this embedding by extension in the following.

The next result is an analogue of Pólya's criterion [11, Th. 4.3.1] for continuous positive definite functions. Our extension also applies to unbounded functions with an integrable singularity at 0.

Theorem 3. *Let $f \in \mathrm{L}^1(\mathbb{R})$ be a function with the following three properties.*

i. *f is locally absolutely continuous on $(0, \infty)$, and $f' \in \mathrm{L}^1_{\mathrm{loc}}((0,\infty))$ has a non-positive, non-decreasing representative.*

ii. *$f(x) = f(-x)$ $(x \in \mathbb{R})$.*

iii. *$f \geq 0$.*

Then $f \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$.

Proof. By Theorem 2, we need only show that the Fourier transform $\hat{f} \geq 0$. Since f is even and real-valued, its Fourier transform $\hat{f}$ is given by

$$\hat{f}(\xi) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(x) \cos(x\,\xi)\, dx \qquad (\xi \in \mathbb{R}),$$

a real-valued, even, bounded function. It is immediate from property iii that $\hat{f}(0) \geq 0$. Hence, it suffices to consider $\xi > 0$ in the following. By property i, f is non-decreasing on $(0, \infty)$. Using this property combined with the facts that f is non-negative and integrable, it follows that

$$\lim_{x\to\infty} f(x) = 0. \tag{9}$$

By the Mean Value Theorem, for any $x > 0$ there is $0 < \xi_x < x$ such that

$$\int_0^x f(y)\, dy = x f(\xi_x).$$

Hence, since f is non-increasing on $(0, \infty)$, it follows that

$$0 \leq x f(x) \leq \int_0^x f(y)\, dy \qquad (x > 0)$$

and consequently

$$\lim_{x\to 0} x f(x) = 0. \tag{10}$$

Since f is locally absolutely continuous on $(0, \infty)$, we can use integration by parts to obtain

$$\int_{x_1}^{x_2} f(x) \cos(x\,\xi)\, dx = \frac{1}{\xi} \left[f(x) \sin(x\,\xi)\right]_{x_1}^{x_2} - \frac{1}{\xi} \int_{x_1}^{x_2} f'(x) \sin(x\,\xi)\, dx$$

$(0 < x_1 < x_2 < \infty)$, where

$$\frac{1}{\xi} \left[f(x) \sin(x\,\xi)\right]_{x_1}^{x_2} = \frac{1}{\xi} f(x_2) \sin(x_2\,\xi) - x_1 f(x_1) \frac{\sin(x_1\,\xi)}{x_1 \xi}.$$

Since $|\sin(x)|$, $|\frac{\sin(x)}{x}| \leq 1$ ($x \in \mathbb{R}$), it follows from (9) and (10) that

$$\lim_{\substack{x_1 \to 0 \\ x_2 \to \infty}} \frac{1}{\xi} \left[f(x) \sin(x\,\xi) \right]_{x_1}^{x_2} = 0.$$

Hence

$$\int_0^\infty f(x) \cos(x\,\xi)\, dx = -\frac{1}{\xi} \int_0^\infty f\,'(x) \sin(x\,\xi)\, dx.$$

Using the same technique as in [23, Eq. 4] we find

$$\begin{aligned}
-\int_0^\infty f'(x) \sin(x\,\xi)\, dx &= -\sum_{j=0}^{\infty} \int_{\frac{2\pi j}{\xi}}^{\frac{2\pi(j+1)}{\xi}} f'(x) \sin(x\,\xi)\, dx \\
&= \frac{1}{\xi} \sum_{j=0}^{\infty} \int_0^\pi \left[f'\left(\frac{2\pi j + \theta}{\xi} + \frac{\pi}{\xi} \right) - f'\left(\frac{2\pi j + \theta}{\xi} \right) \right] \sin(\theta)\, d\theta. \qquad (11)
\end{aligned}$$

Since $\sin(\theta) \geq 0$ on $[0, \pi]$ and f' is non-decreasing, it follows that

$$\int_0^\infty f(x) \cos(x\,\xi)\, dx = -\frac{1}{\xi} \int_0^\infty f'(x) \sin(x\,\xi)\, dx \geq 0.$$

□

Up to this point, we stipulated that the (generalised) positive definite functions must be in $\mathrm{L}^1(\mathbb{R})$. This assumption ensures both the existence of the integral (6) for $\phi \in \mathrm{L}^2(\mathbb{R})$ and the pointwise existence of $\hat{f}$. In the following we show that the generalised definition of positive definiteness can be localised, extending it from $\mathrm{L}^1(\mathbb{R})$ to functions in $\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R})$ or in $\mathrm{L}^1(I)$ for some bounded interval I.

Let $I = [a, b] \subset \mathbb{R}$ be a closed, bounded interval. Let $f \in \mathrm{L}^1([-|I|, |I|])$, where $|I| = b - a$ denotes the length of the interval I. Similarly to Lemma 1, for any $\phi \in \mathrm{L}^2(I)$,

$$\int_{\mathbb{R}} \int_{\mathbb{R}} f(x - y) \phi(x) \overline{\phi(y)}\, dx dy = \int_{-|I|}^{|I|} f(z)\, \phi * \phi^*(z)\, dz, \qquad (12)$$

since $\phi * \phi^*$ has support in $[-|I|, |I|]$. The existence of the integral is guaranteed by the fact that $f \in \mathrm{L}^1([-|I|, |I|])$. By Theorem 2, if the Fourier transform of $f\chi_{[-|I|,|I|]}$ is non-negative, then $f\chi_{[-|I|,|I|]} \in \mathrm{P}(\mathrm{L}^2(\mathbb{R})) \subset \mathrm{P}(\mathrm{L}^2(I))$, which in turn shows the non-negativity of the integral in (12).

The next result is a local variant of Theorem 3, based on the natural embedding of $\mathrm{L}^p(I)$ into $\mathrm{L}^p(\mathbb{R})$. We need a further technical condition at the end-point of the interval.

Corollary 6. *Let $I = [a, b] \subset \mathbb{R}$ be any closed, bounded interval, and $|I| = b - a$ its length. Let $f \in \mathrm{L}^1([-|I|, |I|])$ be a function with the following properties.*

i. *f is locally absolutely continuous on $(0, |I|]$, and $f' \in \mathrm{L}^1_{\mathrm{loc}}((0, |I|])$ has a non-positive, non-decreasing representative.*

ii. $f(x) = f(-x)$ $(x \in [-|I|, |I|])$.

iii. $f(x) \geq 0$ $(x \in [-|I|, |I|])$.

iv. $f(|I|) = 0$ *if* $f'(|I|) = 0$.

Then $f \in \mathrm{P}(\mathrm{L}^2(I))$.

Proof. Define

$$\tilde{f}(x) = \begin{cases} f(x) & \text{if } |x| \leq |I| \\ f(|I|)\, e^{(|x|-|I|)\, f'(|I|)/f(|I|)} & \text{otherwise} \end{cases}$$

if $f(|I|) \neq 0$; if $f(|I|) = 0$, we set $\tilde{f}(x) = 0$ for $|x| > |I|$.

Then the function $\tilde{f}$ satisfies the hypotheses of Theorem 3, and hence is an element of $\mathrm{P}(\mathrm{L}^2(\mathbb{R})) \subset \mathrm{P}(\mathrm{L}^2(I))$. Moreover, $\tilde{f}(x) = f(x)$ $(x \in [-|I|, |I|])$, so $f \in \mathrm{P}(\mathrm{L}^2(I))$. □

Remark. If $f'(|I|) = 0$ and $f(|I|) \neq 0$, then it is not possible to find an extension of the function f from $[-|I|, |I|]$ to the whole real line which is continuous, integrable and has a derivative with a non-decreasing representative.

A function $f : (0, \infty) \to [0, \infty)$ is *completely monotone* if $f \in \mathrm{C}^\infty((0, \infty))$ and

$$(-1)^n\, f^{(n)} \geq 0 \ \text{ on } (0,\, \infty)$$

for all $n \in \mathbb{N}_0$ [15, Def. 1.3]. In particular, any completely monotone function is non-negative and non-increasing. The family of all completely monotone functions is denoted by CM. Completely monotone functions can be bounded or unbounded at zero. If f is a bounded completely monotone function, then it can be extended continuously to $[0,\, \infty)$ by taking $f(0) := f(0+) = \lim_{x \to 0} f(x)$ [15, p. 28].

The following theorem belongs to Schoenberg (along with a number of other theorems on classically positive definite functions, e.g. [15, Prop. 4.4], [15, Th. 12.14], [1, Th. 1.6]). Note that positive definite functions on $\mathbb{R}^d$ are defined by property (1) with $x_1, \ldots, x_n \in \mathbb{R}^d$.

Theorem 4. *A function* $\psi : [0, \infty) \to [0, \infty)$ *is a bounded completely monotone function if and only if for all* $d \in \mathbb{N}$, *the function* $f = \psi(\|\cdot\|^2) : \mathbb{R}^d \to [0, \infty)$ *is continuous and positive definite* [18, Th. 3].

In particular, bounded completely monotone functions with a squared argument are continuous and classically positive definite in the one-dimensional case $d = 1$. The following result generalizes this observation to potentially unbounded completely monotone functions.

Corollary 7. *Let* $f \in$ CM, *and* $g(x) = f(x^2)$ $(x > 0)$. *If* $g \in \mathrm{L}^1(\mathbb{R})$, *then* $g \in \mathrm{P}(\mathrm{L}^2(\mathbb{R}))$.

Proof. By [15, Th. 1.4], f is the Laplace transform of a non-negative measure μ on $[0,\infty)$. That is, for any $x>0$,

$$f(x)=\int_{[0,\infty)} e^{-xt}\,\mu(dt).$$

By the Fubini theorem, for any $\xi\in\mathbb{R}$,

$$\hat{g}(\xi)=\frac{1}{\sqrt{2\pi}}\int_{[0,\infty)}\int_{\mathbb{R}} e^{-x^2t}e^{-ix\xi}\,dx\,\mu(dt)=\int_{[0,\infty)}\frac{1}{\sqrt{2t}}e^{-\xi^2/(4t)}\mu(dt)\geq 0.$$

Thus, $g\in\mathrm{P}(\mathrm{L}^2(\mathbb{R}))$ by Theorem 2. $\square$

We remark that the result of squaring, or taking the square root of, the argument in a completely monotone function will in general not be a completely monotone function.

If we do not square the argument, but just extend the completely monotone function to an even function on the line, then the resulting function will satisfy the hypotheses of Theorem 3, yielding the following Corollary 8, which is similar to Corollary 7. However, the function g of Corollary 7, with a squared argument, does not satisfy property i. in Theorem 3, since $g'(x)=2xf'(x^2)$ is not non-decreasing on $(0,\infty)$; for this reason Corollary 7 above cannot be obtained in this simple way.

Corollary 8. *Let $f\in\mathrm{CM}$. If $g=f(|\cdot|)\in\mathrm{L}^1(\mathbb{R})$, then $g\in\mathrm{P}(\mathrm{L}^2(\mathbb{R}))$.*

Moreover, we have the following localised versions.

Corollary 9. *Let $I\subset\mathbb{R}$ be any closed interval. Let $f\in\mathrm{CM}$ be non-constant. If $g=f(|\cdot|)\in\mathrm{L}^1([-|I|,|I|])$, then $g\in\mathrm{P}(\mathrm{L}^2(I))$.*

Proof. If $f\in\mathrm{CM}$, then by [15, Remark 1.5] $f^{(n)}(x)\neq 0$ for all $n\geq 1$ and all $x>0$ unless f is identically constant. Thus g satisfies the hypotheses of Corollary 6. $\square$

Corollary 10. *Let $f\in\mathrm{CM}$ be non-constant. If $g=f(|\cdot|)\in\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R})$, then $g\in\mathrm{P}(\mathrm{L}^2_0(\mathbb{R}))$.*

Proof. For any $\phi\in\mathrm{L}^2_0(\mathbb{R})$,

$$\int_{\mathbb{R}}\int_{\mathbb{R}} g(x-y)\phi(x)\overline{\phi(y)}\,dxdy=\int_{\mathrm{I}}\int_{\mathrm{I}} g(x-y)\phi(x)\overline{\phi(y)}\,dxdy, \tag{13}$$

where I includes the compact support of ϕ. Since $g\in\mathrm{L}^1_{\mathrm{loc}}(\mathbb{R})$, it follows that $g\in\mathrm{L}^1([-|I|,|I|])$, and by Corollary 9 the integral in (13) is non-negative. $\square$

Completely monotone functions can be obtained as derivatives of Bernstein functions [15, p.18]. Taking functions f_i from the list of Bernstein functions in [15, Chapter 15], the following derived functions $g_i=f_i'(|\cdot|)$ are elements of

$\mathrm{P}(\mathrm{L}_0^2(\mathbb{R})) \setminus \mathrm{P}_\mathrm{C}$ by Corollary 10.

$$
\begin{aligned}
g_1(x) &= |x|^{-\alpha},\ 0<\alpha<1;\\
g_8(x) &= |x|^{\alpha-1}/(1+|x|)^{\alpha+1},\ 0<\alpha<1;\\
g_{11}(x) &= \Big(\alpha|x|^{\alpha-1}(1-|x|^{\beta}) - \beta|x|^{\beta-1}(1-|x|^{\alpha})\Big)/(1-|x|^{\alpha})^2,\\
&\quad 0<\alpha<\beta<1\,;\\
g_{16}(x) &= \left(\alpha_1|x|^{-\alpha_1-1}+\ldots+\alpha_n|x|^{-\alpha_n-1}\right)/\left(|x|^{-\alpha_1}+\ldots+|x|^{-\alpha_n}\right)^2,\\
&\quad 0\le\alpha_1,\ldots,\alpha_n\le 1;\\
g_{18,19}(x) &= \Big(1\pm(2a\sqrt{|x|}-1)e^{-2a\sqrt{|x|}}\Big)/\sqrt{|x|},\ a>0;\\
g_{23}(x) &= |x|\,(1+1/|x|)^{1+|x|}\log(1+1/|x|) \qquad\qquad (x\in\mathbb{R}\setminus\{0\}).
\end{aligned}
$$

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