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# On the Extremal Rays of the Cone of Positive, Positive Definite Functions

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**Abstract** The aim of this paper is to investigate the cone of non-negative, radial, positive-definite functions in the set of continuous functions on $\mathbb{R}^d$. Elements of this cone admit a Choquet integral representation in terms of the extremals. The main feature of this article is to characterize some large classes of such extremals. In particular, we show that there are many other extremals than the Gaussians, thus disproving a conjecture of G. Choquet, and that no reasonable conjecture can be made on the full set of extremals.

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The last feature of this article is to show that many characterizations of positive definite functions available in the literature are actually particular cases of the Choquet integral representations we obtain.

**Keywords** Choquet integral representation · Extremal ray generators · Positive definite functions

**Mathematics Subject Classification (2000)** 42A82

## 1 Introduction

Positive definite functions appear in many areas of mathematics, ranging from number theory to statistical applications. Since Bochner's work, these functions are known to be characterized as having a non-negative Fourier transform.

Before going on, let us first fix some notations. We will define the Fourier transform of a function $f \in L^1(\mathbb{R}^d)$ by

$$\mathcal{F}_d f(\xi) = \widehat{f}(\xi) = \int_{\mathbb{R}^d} f(x) e^{2i\pi\langle x,\xi\rangle}\,\mathrm{d}x$$

and extend this definition both to bounded measures on $\mathbb{R}^d$ and to $L^2(\mathbb{R}^d)$ in the usual way. Here $\langle\cdot,\cdot\rangle$ is the scalar product on $\mathbb{R}^d$ and $|\cdot|$ is the Euclidean norm.

A continuous function $f$ of $\mathbb{R}^n$ is said to be *positive definite* if, for every integer $n$, for all $x_1,\dots,x_n \in \mathbb{R}^d$, the $n\times n$ matrix $[f(x_j-x_k)]_{1\le j,k\le n}$ is positive definite, that is, if

$$\sum_{j,k=1}^{n} c_j\overline{c_k} f(x_j-x_k) \ge 0 \quad \text{for all } c_1,\dots,c_n \in \mathbb{C}. \tag{1}$$

Then Bochner's theorem [8] shows that $f$ is positive definite if and only if $f=\widehat{\mu}$ for some positive bounded Radon measure on $\mathbb{R}^d$ (a probability measure if we further impose $f(0)=1$). There are many proofs of Bochner's theorem, the nearest to the subject of this paper being based on the Choquet Representation theorem, due to Bucy and Maltese [12], see also [4, 14, 15, 20, 39]. Let us sketch the main features of these proofs, and thereby also some definitions (details may be found in the previous references). An element $f$ of a cone $\Omega \ni f$ is an extremal ray generator of $\Omega$ (or simply an extremal) if $f=f_1+f_2$ with $f_1,f_2\in\Omega$ implies $f_1=\lambda f$, $f_2=\mu f$, $\lambda,\mu\ge 0$. The first step in the proof of Bochner's theorem is then to show that the characters $e^{2i\pi\langle x,\xi\rangle}$ are the only extremal rays of the cone of positive definite functions. The second step is to show that the cone of positive definite functions on $\mathbb{R}^d$ is well capped, i.e. is the union of caps (compact, convex subsets $C$ of $\Omega$ such that $\Omega\setminus C$ is still convex). At this stage, there is a slight subtlety. In order to prove compactness, the notion of positive definiteness is first extended to $L^\infty$-functions. Bucy and Maltese then proved that the cone of positive definite $L^\infty$-functions endowed with the $\sigma(L^\infty,L^1)$-topology is a well-capped cone. It then follows from the work of Choquet that every element of such a cone is an integral over extreme points with respect to a conical measure. Finally, one checks that this integral representation of positive definite functions is the same as taking the Fourier transform of a measure. As a corollary one then obtains that the $L^\infty$-positive definite functions are the same as the continuous positive definite functions as defined above.

Let us mention that positive definite functions may also be considered on more general locally compact Abelian groups (see e.g. [20, Chap. 3] and [34, 35] for some recent work in that context). In this case, Bochner's theorem has been proved via Choquet theory in [1].

Let us now note that Bochner's theorem, though being powerful when one wants to construct positive definite functions, may be difficult to use in practice. This mainly comes from the fact that explicit computations of Fourier transforms are generally impossible. For instance, it is not known precisely for which values of $\lambda$ and $\kappa$ the function $(1-|x|^\lambda)_+^\kappa$ is positive definite on $\mathbb{R}^d$. This problem is known as the Kuttner-Golubov problem and we refer to [25] for more details and the best known results to date. To overcome this difficulty, one seeks concrete and easily checkable criteria that guarantee that a function is positive definite. The most famous such criterion is due to Pólya which shows that a bounded continuous even function on $\mathbb{R}$ which is convex on $[0,+\infty)$, is positive definite. More evolved criteria may be found in the literature (see Sect. 5 for more details).

As it turns out, the functions so characterized are not only positive definite but also non-negative. We will call such functions *positive positive definite*. Such functions appear in many contexts. To give a few examples where the reader may find further references, let us mention various fields such as approximation theory [13], spatial statistics [9], geometry of Banach spaces [36], and physics [26]. Despite a call to study such functions by P. Lévy in [37] they seem not to have attracted much attention so far. To our knowledge, there are only two papers specifically devoted to the subject in the literature: [23] which is motivated by applications in physics and the (unpublished) paper [10] which is motivated by problems in number theory.

Before going on with the description of the main features of this paper, we will need some further notations. First, let us recall that a function is radial if it is of the form $f(x)=\varphi(|x|)$. For $d\geq 1$ we define $\mathcal{C}_r(\mathbb{R}^d)$ to be the space of radial continuous functions, and we stress the fact that in the sequel we will only consider *radial* functions in dimensions higher than 1. Now, let

$$\Omega_d=\{f\in\mathcal{C}_r(\mathbb{R}^d): f \text{ is positive definite}\}$$

and $\Omega_d^+=\{f\in\Omega_d : f\geq 0\}$. Note that in dimension 1, a positive definite function is even, so there is no restriction when considering radial functions in this case.

Next, $\Omega_d^+$ is a closed convex sub-cone of $\Omega_d$ in $\mathcal{C}_r(\mathbb{R}^d)$. For $f\in\Omega_d^+$, we denote by $I(f)=\Omega_d^+\cap(f-\Omega_d^+)$ the *interval* generated by $f$. Then $f$ is an *extremal ray generator* if $I(f)=\{\lambda f:\ 0\leq\lambda\leq 1\}$. As the cone $\Omega_d$ is well-capped, so is $\Omega_d^+$.[1] Therefore, Choquet Theory applies and every positive positive definite function admits an integral representation over extremals. It is therefore a natural task to determine the extremals of $\Omega_d^+$.

[1] Here again, one first considers the cone as a sub-cone of the cone of $L^\infty$-positive definite functions endowed with the weak $*\ \sigma(L^1,L^\infty)$ topology on $L^\infty$.

We are unfortunately unable to fulfill this task completely. One difficulty is that among the extremals of the cone of positive definite functions, only the trivial character 1 is still in the cone of positive positive definite functions and is of course an extremal of it. We are nevertheless able to describe large classes of extremals. One such class is included in the compactly supported extremals of $\Omega_d^+$. In this case, we show that if an element of $\Omega_d^+$ with compact support has a Fourier transform whose holomorphic extension to $\mathbb{C}$ has only real zeroes, then this element is an extremal ray generator. One would be tempted to conjecture that this describes all compactly supported extremals, but we show that this is not the case. Nevertheless, this theorem allows us to show that many examples of functions used in practice are extremals, as for instance the functions $(1-|x|^2)_+^\alpha * (1-|x|^2)_+^\alpha$ for suitable $\alpha$'s.

The next class of functions we investigate is that of Hermite functions, that is, functions of the form $P(x)e^{-\lambda x^2}$, $P$ a polynomial. This is a natural class to investigate since the elements of the intervals they generate consist of functions of the same form. This will be shown as a simple consequence of Hardy's Uncertainty Principle. Further, a conjecture in the folklore [27] (attributed to G. Choquet although P. Lévy may be another reasonable source of the conjecture) states the following:

**Conjecture** (Choquet) *The only extremals in the cone of positive and positive definite functions on* $\mathbb{R}$ *are the Gaussians.*

This conjecture is false, as our results on compactly supported extremals show. We will construct more counter-examples by describing precisely the positive positive definite functions of the form $P(x)e^{-\pi x^2}$ where $P$ is a polynomial of degree 4 and showing that this class contains extremal ray generators. This further allows us to construct extremals of the form $P(x)e^{-\pi x^2}$ with $P$ polynomials of arbitrary high degree.

Finally, we show that most (sufficient) characterizations of positive definite functions actually characterize positive positive definite functions and are actually particular cases of Choquet representations. More precisely, it is easy to see that if $\varphi$ is an extremal ray generator in $\Omega_d^+$ then so is $\varphi_t(x) = \varphi(tx)$. It follows that

$$\int_0^{+\infty} \varphi_t \, \mathrm{d}\mu(t) \tag{2}$$

is a positive positive definite function (for suitable $\mu$) that is obtained by a Choquet representation with a measure supported on the family of extremals $\{\varphi_t\}$. For instance:

- As a particular case of our theorem concerning compactly supported functions, we obtain that the function $\varphi(x) = (1-|x|)_+$ is extremal. Pólya's criterium may be seen as a characterization of those functions which may be written in the form (2).
- A criterium for deciding which functions may be written in the form (2) with $\varphi(x) = (1-|x|^2)_+ * (1-|x|^2)_+$ has been obtained by Gneiting.

The article is organized as follows. In the next section, we gather preliminaries on positive definite functions. We then turn to the case of compactly supported functions in Sect. 3, followed by the case of Hermite functions. We then devote Sect. 5 to link our results with various criteria available in the literature. We conclude the paper with some open questions.

## 2 Preliminaries

### 2.1 Basic Facts

**Fact 1** (Invariance by scaling) *Let $f$ be a continuous function and $\lambda > 0$. We write $f_\lambda(x) = f(\lambda x)$. Then $f \in \Omega_d^+$ if and only if $f_\lambda \in \Omega_d^+$. Moreover $f$ is an extremal ray generator if and only if $f_\lambda$ is extremal.*

Another consequence is the following lemma:

**Lemma 2.1** *Let $\omega \in \Omega_d^+$ and $\nu$ be a positive bounded measure on $(0, +\infty)$. Define*

$$F(x) = \int_0^{+\infty} \omega(x/t)\,\mathrm{d}\nu(t).$$

*Then $F \in \Omega_d^+$. Moreover, write $\omega(x) = \omega_0(|x|)$ and assume that $\omega_0$ is non-increasing on $(0, +\infty)$ and (strictly) decreasing in a neighborhood of 0. Then $F$ is an extremal ray generator if and only if $\omega$ is an extremal ray generator and $\nu = \delta_a$ is a Dirac mass for some $a \in (0, +\infty)$.*

*Proof* Note that the fact that $F$ is continuous follows from Lebesgue's theorem since $\omega$ is bounded and continuous. It is then also obvious that $F$ is positive and positive definite.

If $\omega$ is an extremal ray generator and $\nu = \delta_a$ then $F(x) = \omega(x/a)$ is clearly an extremal ray generator. It is also immediate that if $\omega$ is not extremal then $F$ is not extremal.

Finally, assume that the support of $\nu$ contains at least 2 points $a < b = a + 3\eta$ and let $\psi$ be a continuous non-increasing function such that $0 \le \psi \le 1$ and $\psi(x) = 1$ on $(0, a + \eta)$ while $\psi = 0$ on $(a + 2\eta, +\infty)$. Define

$$F_1(x) = \int_0^{+\infty} \omega(x/t)\psi(t)\,\mathrm{d}\nu(t) \quad \text{and} \quad F_2(x) = \int_0^{+\infty} \omega(x/t)\big(1 - \psi(t)\big)\,\mathrm{d}\nu(t).$$

The measures $\psi(t)\,\mathrm{d}\nu(t)$ and $(1 - \psi(t))\,\mathrm{d}\nu(t)$ are bounded, so that $F_1, F_2$ are continuous, $F_1$ and $F_2$ are positive positive definite, $F = F_1 + F_2$.

Assume now towards a contradiction that $F_1 = \lambda F$ with $0 \le \lambda \le 1$. From the assumption on $\psi$, we easily deduce that $0 < \lambda < 1$. Let $t_0$ be a solution of $\psi(t) = \lambda$. From $\int_0^{+\infty} \omega(x/t)(\psi(t) - \lambda)\,\mathrm{d}\nu(t) = 0$ we get that

$$\int_0^{t_0} \omega(x/t)\big(\psi(t) - \lambda\big)\,\mathrm{d}\nu(t) = \int_{t_0}^{+\infty} \omega(x/t)\big(\lambda - \psi(t)\big)\,\mathrm{d}\nu(t). \tag{3}$$

In particular, for $x=0$, we obtain

$$\int_0^{t_0} \big(\psi(t)-\lambda\big)\,\mathrm{d}\nu(t) = \int_{t_0}^{+\infty} \big(\lambda-\psi(t)\big)\,\mathrm{d}\nu(t).$$

Now, $\chi_{(0,t_0)}(\psi(t)-\lambda)\,\mathrm{d}\nu(t)$ and $\chi_{(t_0,+\infty)}(\lambda-\psi(t))\,\mathrm{d}\nu(t)$ are positive non-zero measures. Then, for $|x_0|>0$ small enough to have that $\omega$ is strictly decreasing on $(0,|x_0|/t_0)$, we get

$$\begin{aligned}
\int_0^{t_0} \omega(x_0/t)\big(\psi(t)-\lambda\big)\,\mathrm{d}\nu(t) &= \int_0^{t_0} \omega_0(|x_0|/t)\big(\psi(t)-\lambda\big)\,\mathrm{d}\nu(t)\\
&\le \omega_0(|x_0|/t_0)\int_0^{t_0} \big(\psi(t)-\lambda\big)\,\mathrm{d}\nu(t)\\
&= \omega_0(|x_0|/t_0)\int_{t_0}^{+\infty} \big(\lambda-\psi(t)\big)\,\mathrm{d}\nu(t)\\
&< \int_{t_0}^{+\infty} \omega_0(|x_0|/t)\big(\lambda-\psi(t)\big)\,\mathrm{d}\nu(t)\\
&= \int_{t_0}^{+\infty} \omega(x_0/t)\big(\lambda-\psi(t)\big)\,\mathrm{d}\nu(t)
\end{aligned}$$

a contradiction, so that $F_1\neq\lambda F$ and $F$ is not an extremal ray generator. □

**Fact 2** (Invariance under products and convolution) *If $f,g\in\Omega_d^+$ then $fg\in\Omega_d^+$. Further, if $f,g$ are also in $L^2$ (say) then $f*g\in\Omega_d^+$.*

*Further if either $f$ or $g$ (resp. $\widehat{f}$ or $\widehat{g}$) does not vanish, then, for $fg$ (resp. $f*g$) to be extremal, it is necessary that both $f$ and $g$ are extremal.*

Indeed, assume that $g$ is not extremal and write $g=g_1+g_2$ with $g_1/g$, $g_2/g$ not constant, then $fg=fg_1+fg_2$. Now, if $fg_1=\lambda fg$ then $g_1=\lambda g$ on the support of $f$.

The converse is unclear and probably false. A possible counter-example may be constructed as follows. Assume there is a compactly supported extremal $f$ such that $f^2$ is also extremal. Without loss of generality, we may assume that $f$ is supported in $[-1,1]$. Let $g=(4\delta_0+\delta_{-4\pi}+\delta_{4\pi})*f$ then $fg=4f^2$ would be extremal but $g$ is not.

## 2.2 Bessel Functions and Fourier Transforms

Results in this section can be found in most books on Fourier analysis, for instance [28, Appendix B].

Let $\lambda$ be a real number with $\lambda>-1/2$. We define the Bessel function $J_\lambda$ of order $\lambda$ on $(0,+\infty)$ by its *Poisson representation formula*

$$J_\lambda(x) = \frac{x^\lambda}{2^\lambda\Gamma(\lambda+\frac12)\Gamma(\frac12)}\int_{-1}^{1} e^{isx}(1-s^2)^\lambda\frac{\mathrm{d}s}{\sqrt{1-s^2}}.$$

Let us define $\mathcal{J}_{-1/2}(x)=\cos x$ and for $\lambda>-1/2$, $\mathcal{J}_\lambda(x):=\frac{J_\lambda(x)}{x^\lambda}$. Then $\mathcal{J}_\lambda$ extends to an even entire function of order 1 and satisfies $\mathcal{J}_\lambda(x)$ real and $\mathcal{J}_\lambda(ix)>0$ for all $x\in\mathbb{R}$. It is also known that $\mathcal{J}_\lambda$ has only real simple zeroes.

As is well-known, if $f$ is a radial function given by $f(x)=f_0(|x|)$, then its Fourier transform is given by

$$\widehat{f}(\xi)=\mathcal{J}_{\frac{d}{2}-1}(f_0)(|\xi|)$$

where

$$\mathcal{J}_\lambda(f_0)(t)=(2\pi)^{\lambda+1}\int_0^{+\infty}f_0(r)\mathcal{J}_\lambda(2\pi rt)r^{2\lambda+1}\,\mathrm{d}r.$$

Bochner's theorem has been extended to radial continuous positive definite functions by Schoenberg [43, p. 816] (see also [45]): a function $\varphi$ is positive definite and radial on $\mathbb{R}^d$, $d\geq 2$ if and only if there exists a positive bounded measure $\mu$ on $(0,+\infty)$ such that $\varphi(x)=\varphi_0(|x|)$ with

$$\varphi_0(r)=r^{-\frac{d}{2}+1}\int_0^{+\infty}J_{\frac{d}{2}-1}(2\pi rs)\,\mathrm{d}\mu(s)=(2\pi)^{\frac{d}{2}-1}\int_0^{+\infty}\mathcal{J}_{\frac{d}{2}-1}(2\pi rs)\,s^{\frac{d}{2}-1}\mathrm{d}\mu(s).$$

For $d=1$ this coincides with Bochner's theorem.

We will also use the following well-known result: denote $|t|_+=t$ or 0 according to $t>0$ or not. Let $m_\alpha(x)=(1-|x|^2)_+^\alpha$. Then

$$\widehat{m_\alpha}(\xi)=\frac{\Gamma(\alpha+1)}{\pi^\alpha}\frac{J_{\frac{d}{2}+\alpha}(2\pi|\xi|)}{|\xi|^{\frac{d}{2}+\alpha}}=2^{\frac{d}{2}+\alpha}\pi^{\frac{d}{2}}\Gamma(\alpha+1)\mathcal{J}_{\frac{d}{2}+\alpha}(2\pi|\xi|).$$

## 3 Compactly Supported Positive Positive Definite Functions

In this section, we consider compactly supported positive positive definite functions. It is natural to look for extremals inside this class of functions because of the following (trivial) lemma:

**Lemma 3.1** *Let $f$ be a continuous radial positive positive definite function with compact support. Then the interval $I(f)$ contains only positive positive definite functions with support included in* supp $f$.

*Moreover, if we write $B(0,a)$ for the smallest ball containing* supp $f$, *i.e.* conv supp $f=B(0,a)$, *and if $f=g+h$ with $g,h\subset I(f)$, then at least one of* conv supp $g$ *and* conv supp $h$ *is $B(0,a)$.*

*Proof* First if $g\in I(f)$ then $0\leq g\leq f$ so that supp $g\subset$ supp $f$.

Next, as $f$ is radial, there exists $a$ such that conv supp $f=B(0,a)$. Assume now that $f=g+h$ with $g,h\in I(f)$. As $g$ (resp. $h$) is radial, the convex hull of its support is a ball and we denote it by $B(0,b)$ (resp. $B(0,c)$). As $g$ and $h$ are both non-negative, the convex hull of the support of $g+h=f$ is then $B(0,\max(b,c))=B(0,a)$ thus the claim. □

We may now prove the following:

**Theorem 3.2** *Let $f \in \mathcal{C}(\mathbb{R}^d)$ be a compactly supported positive positive definite radial function. Write $f(x) = f_0(|x|)$ where $f_0$ is a compactly supported function on $\mathbb{R}_+$ so that $\mathcal{J}_{\frac{d}{2}-1}(f_0)$ extends analytically to $\mathbb{C}$.*

*Assume that $\mathcal{J}_{\frac{d}{2}-1}(f_0)$ has only real zeroes, then $f$ is an extreme ray generator in the cone of continuous positive positive definite radial functions.*

*Moreover, assume that $\mathcal{J}_{\frac{d}{2}-1}(f_0)$ has only a finite number $N$ of non-real zeroes, and let $g \in I(f)$. If we write $g = g_0(|x|)$, then $\mathcal{J}_{\frac{d}{2}-1}(g_0)$ has at most $N$ non-real zeroes.*

*Proof* Let us write $f = g + h$ with $g, h$ radial positive positive definite functions. Then $g$ and $h$ are also compactly supported.

Write $g(x) = g_0(|x|)$ and $h(x) = h_0(|x|)$. It follows that $\mathcal{J}_{\frac{d}{2}-1}(f_0)$, $\mathcal{J}_{\frac{d}{2}-1}(g_0)$ and $\mathcal{J}_{\frac{d}{2}-1}(h_0)$ all extend to entire functions of order 1. From Hadamard's factorization theorem, we may write $\mathcal{J}_{\frac{d}{2}-1}(f_0)$ as

$$\mathcal{J}_{\frac{d}{2}-1}(f_0)(z) = z^k e^{az+b} \prod_{\zeta \in \mathcal{Z}(f)} \left(1 - \frac{z}{\zeta}\right) \exp \frac{z}{\zeta} \tag{4}$$

where $\mathcal{Z}(f)$ is the set of non-zero zeroes of $\mathcal{J}_{\frac{d}{2}-1}(f_0)$. Let us further note that

(i) $\mathcal{J}_{\frac{d}{2}-1}(f_0)$ is real if $z \in \mathbb{R}$, thus $a, b \in \mathbb{R}$ and if $\zeta \in \mathcal{Z}(f)$ then $\overline{\zeta} \in \mathcal{Z}(f)$;
(ii) $\mathcal{J}_{\frac{d}{2}-1}(f_0)$ is non-negative if $z \in \mathbb{R}$, thus real zeroes are of even order;
(iii) $\mathcal{J}_{\frac{d}{2}-1}(f_0)(0) = \widehat{f}(0) = \int f \neq 0$ since $f \geq 0$ thus $k = 0$;
(iv) $\mathcal{J}_{\frac{d}{2}-1}(f_0)$ is even thus if $\zeta \in \mathcal{Z}(f)$ then $-\zeta \in \mathcal{Z}(f)$ and $a = 0$.

We may thus simplify (4) to $\mathcal{J}_{\frac{d}{2}-1}(f_0)(z) = \widehat{f}(0) E_f(z) P_f(z)$ with

$$E_f(z) = \prod_{\zeta \in \mathcal{Z}_+(f)} \left(1 - \frac{z^2}{\zeta^2}\right)^2$$

where $\mathcal{Z}_+(f) = \mathcal{Z}(f) \cap (0, +\infty)$ and

$$P_f(z) = \prod_{\zeta \in \mathcal{Z}_Q(f)} \left(1 - \frac{z^2}{\zeta^2}\right)\left(1 - \frac{z^2}{\overline{\zeta}^2}\right)$$

where $\mathcal{Z}_Q(f) = \{\zeta \in \mathcal{Z}(f) : \operatorname{Re}\zeta > 0 \ \& \ \operatorname{Im}\zeta > 0\}$. Similar expressions hold for $\mathcal{J}_{\frac{d}{2}-1}(g_0)$ and $\mathcal{J}_{\frac{d}{2}-1}(h_0)$. It should also be noticed that both $E_f$ and $P_f$ are non-negative on the real and the imaginary axes.

Now, let us assume that $\mathcal{J}_{\frac{d}{2}-1}(f_0)$ has only finitely many non-real zeroes, so that $P_f$ is a polynomial. In particular, there exists an integer $N$ and a constant $C$ such that $|P_f(z)| \leq C(1 + |z|)^N$.

As $\mathcal{J}_{\frac{d}{2}-1}(f_0) = \mathcal{J}_{\frac{d}{2}-1}(g_0) + \mathcal{J}_{\frac{d}{2}-1}(h_0)$ with $\mathcal{J}_{\frac{d}{2}-1}(h_0) \geq 0$, we get $0 \leq \mathcal{J}_{\frac{d}{2}-1}(g_0)(z) \leq \mathcal{J}_{\frac{d}{2}-1}(f_0)(z)$ for $z$ *real*. It follows that $\mathcal{Z}_+(f) \subset \mathcal{Z}_+(g)$, with multiplicity. Thus, we may partition the multiset $\mathcal{Z}_+(g) = \mathcal{Z}_+(f) \cup \mathcal{Z}'(g)$.

From Hadamard's factorization, it follows that

$$\mathcal{J}_{\frac{d}{2}-1}(g_0)(z)=\widehat{g}(0)E_f(z)\prod_{\zeta\in\mathcal{Z}'(g)}\left(1-\frac{z^2}{\zeta^2}\right)\cdot P_g(z).$$

So, we have written $\mathcal{J}_{\frac{d}{2}-1}(g_0)(z)=G(z)E_f(z)$ where $G$ is an entire function of order at most 1. Note that $0\le\mathcal{J}_{\frac{d}{2}-1}(g_0)(x)\le\mathcal{J}_{\frac{d}{2}-1}(f_0)(x)$, so that $0\le|G(x)|\le C(1+|x|)^N$ for $x$ real.

Further, from the positivity of $f$ and $g$,

$$\begin{aligned}0<\mathcal{J}_{\frac{d}{2}-1}(g_0)(it)&=\int_{B(0,a)}g(x)e^{2\pi tx}\,\mathrm{d}x\le\int_{B(0,a)}f(x)e^{2\pi tx}\,\mathrm{d}x\\&=\mathcal{J}_{\frac{d}{2}-1}(f_0)(it).\end{aligned}\tag{5}$$

It follows that $|G(z)|$ is also bounded by $C(1+|z|)^N$ on the imaginary axis. By Phragmén-Lindelöf's Principle $G$ is bounded by $2^NC(1+|z|)^N$ over each of the four quadrants $Q_{\varepsilon_1,\varepsilon_2}=\{\varepsilon_1\mathrm{Re}\,z\ge0\ \&\ \varepsilon_2\mathrm{Im}\,z\ge0\}$, $\varepsilon_1=\pm1,\varepsilon_2=\pm1$. From Liouville's Theorem, we thus get that $G$ is a polynomial of degree at most $N$.

In particular, if $N=0$, then $G$ is a constant and $\mathcal{J}_{\frac{d}{2}-1}(g_0)=\lambda\mathcal{J}_{\frac{d}{2}-1}(f_0)$ thus $g=\lambda f$. It follows that $h=(1-\lambda)f$, and $f$ is an extremal ray generator. □

*Remark* Note that in the course of the proof we have shown that if the Fourier transform $\widehat{f}$ of a compactly supported positive positive definite function $f$ has a non real zero $\zeta$, then $\zeta$ is not purely imaginary (see (5)) and $-\zeta$, $\overline{\zeta}$, $-\overline{\zeta}$ are also zeroes of $\widehat{f}$.

It should be noted that checking whether a particular function is an extremal positive positive definite function may be difficult in practice. Nevertheless, we will now give a few examples.

*Example* Let us consider the characteristic (indicator) function $\chi_{[-1,1]}$ of the interval $[-1,1]$ in $\mathbb{R}$. Then $p(x):=\chi_{[-1,1]}*\chi_{[-1,1]}$ is an extremal ray generator since its Fourier transform is $\widehat{p}(\xi)=(\frac{\sin 2\pi\xi}{\pi\xi})^2$.

The celebrated positive definiteness criteria of Pólya characterizes those functions that may be written in the form $\int p(x/r)\,\mathrm{d}\mu(r)$ with $\mu$ a positive measure (see Sect. 5.1).

Further examples are obtained by convolving $p$'s:

$$\chi_{[-r_1/2,r_1/2]}*\chi_{[-r_1/2,r_1/2]}*\cdots*\chi_{[-r_k/2,r_k/2]}*\chi_{[-r_k/2,r_k/2]}.$$

Another class of examples is given by the following:

**Corollary 3.3** *For $\alpha>-1/2$ define the function $m_\alpha$ on $\mathbb{R}^d$ by*

$$m_\alpha(x)=(1-|x|^2)_+^\alpha:=\begin{cases}(1-|x|^2)^\alpha & \textit{if } |x|<1,\\ 0 & \textit{otherwise}.\end{cases}$$

*Then, $m_\alpha * m_\alpha$ is a continuous positive positive definite function that is an extremal ray generator.*

This covers the previous example and extends it to higher dimension since $m_0$ is the characteristic (indicator) function of the unit ball of $\mathbb{R}^d$.

*Remark* If we were considering positive definite tempered distributions, then this result stays true for $\alpha > -1$.

*Proof* First of all, note that if $\alpha \geq 0$, $m_\alpha \in L^\infty$ and for $-1 < \alpha < 0$, $m_\alpha \in L^p$ for all $\alpha > -1/p$. It follows that $m_\alpha * m_\alpha$ is well defined, has compact support and is continuous for all $\alpha > -1/2$.

Further, as is well-known (see e.g. [28, Appendix B5]):

$$\widehat{m_\alpha}(\xi) = \frac{\Gamma(\alpha+1)}{\pi^\alpha} \frac{J_{d/2+\alpha}(2\pi|\xi|)}{|\xi|^{d/2+\alpha}}.$$

It follows that the Fourier transform of $m_\alpha * m_\alpha$ is given by

$$\widehat{m_\alpha * m_\alpha}(\xi) = \frac{\Gamma(\alpha+1)^2}{\pi^{2\alpha}} \frac{J_{d/2+\alpha}(2\pi|\xi|)^2}{|\xi|^{d+2\alpha}}.$$

But, from a theorem of Hurwitz [32] (see [48, 15.27, p. 483]), $J_{d/2+\alpha}$ has only positive zeroes since $d/2+\alpha > -1$. The corollary thus follows from the previous theorem. □

*Example* A particular case of the previous result is that the function $w(x) := m_1(x) * m_1(x) = (1-x^2)_+ * (1-x^2)_+$ on $\mathbb{R}$ is an extremal ray generator. The function $w$ has been introduced in the study of positive definite functions by Wu [52] in the context of radial basis function interpolation. A simple criteria for writing a function in the form $\int w(x/r)\,\mathrm{d}\mu(r)$ with $\mu$ a positive bounded measure has been recently obtained by Gneiting [24] (see Sect. 5.2).

Further examples are then obtained by taking scales $w_r$ of $w$ and convolving several $w_r$'s together:

$$(1-x^2/r_1^2)_+ * (1-x^2/r_1^2)_+ * \cdots * (1-x^2/r_k^2)_+ * (1-x^2/r_k^2)_+.$$

*Remark* When $\lambda \to \infty$ we have $m_\lambda(\sqrt{\pi}x/\sqrt{\lambda}) \to e^{-\pi x^2}$ pointwise, in $L^2$, and uniformly on compact sets.

It would be tempting to conjecture that every compactly supported extreme ray generator is covered by Theorem 3.2, i.e. it is of the form that its Fourier transform has only real zeroes. Nevertheless, this is not the case:

**Proposition 3.4** *There exists a continuous compactly supported extreme ray generator $f$ of $\Omega_1^+$ such that $\widehat{f}$ has non-real zeroes.*

*Proof* Consider $\varphi(x)=(1-x^2)_+^2*(1-x^2)_+^2$. A cumbersome computation (by computer) shows that

$$\varphi(x)=\begin{cases}\frac{1}{630}(2-x)^5(x^4+10|x|^3+36x^2+40|x|+16) & \text{if } |x|<2,\\ 0 & \text{otherwise.}\end{cases}$$

Let $r>0$ and $0<\theta<\pi/2$ and $\zeta=\frac{r}{2\pi}e^{i\theta}$, let us define $f_{r,\theta}=f_\zeta$ by

$$\begin{aligned}\widehat{f_\zeta}(\xi)&=\left(1-\frac{\xi}{\zeta}\right)\left(1+\frac{\xi}{\zeta}\right)\left(1-\frac{\xi}{\bar\zeta}\right)\left(1+\frac{\xi}{\bar\zeta}\right)\widehat{\varphi}(\xi)\\ &=\left(1+\frac{2\cos 2\theta}{r^2}(2i\pi\xi)^2+\frac{1}{r^4}(2i\pi\xi)^4\right)\widehat{\varphi}(\xi).\end{aligned}\tag{6}$$

Then $f_\zeta$ is positive definite.

Further, as $\varphi$ is smooth, and as $\widehat{\partial^k\varphi}(\xi)=(2i\pi\xi)^k\widehat{\varphi}(\xi)$ we get that

$$f_\zeta(x)=\left(1+\frac{2\cos 2\theta}{r^2}\partial^2+\frac{1}{r^4}\partial^4\right)\varphi(x).$$

The computations are easily justified by the fact that $\varphi$ is of class $\mathcal{C}^4$. Note that, for $|x|\le 2$,

$$\varphi''(x)=\frac{4}{105}(3x^4+18|x|^3+30|x|^2-12|x|-8)(2-x)^3$$

and

$$\varphi^{(4)}(x)=\frac{8}{5}(3x^4+6|x|^3-8x^2-16|x|+8)(2-x).$$

We will now take $\theta=\pi/4$. Actually, we believe that for every $0<\theta<\pi/2$ there is a unique $r$ such that $f_\zeta$ is extremal.

We then have

$$f_\zeta(x)=\varphi(x)+\varphi^{(4)}(x)/r^4.$$

It is not hard to see that $\varphi$ is decreasing and positive on $(0,2)$ and that $\varphi^{(4)}$ is decreasing on $(0,\sqrt{2-2/\sqrt{3}})$ and on $(\sqrt{2+2/\sqrt{3}},2)$ increasing on $(\sqrt{2-2/\sqrt{3}},\sqrt{2+2/\sqrt{3}})$, positive on $(0,x_1)\cup(x_2,2)$ and negative on $(x_1,x_2)$ where $x_1=0.441\dots$ and $x_2=1.462\dots$. In particular, for $r$ big enough ($r=4$ will do), $f_{r,\pi/4}$ is positive on $(0,2)$ and for $r$ small enough ($r=3$ will do), $f_{r,\pi/4}$ has two zeroes on $(0,2)$. Therefore, there exists a unique $r$ such that $f_{r,\pi/4}$ has exactly one double zero on $(0,2)$. A numerical computation shows that $r\simeq 3.342775$. Let us denote this zero by $x_\zeta$. A computer computation shows that $x_\zeta\simeq 1.303$.

We will need a bit more information. Let $\xi=\frac{\rho}{2\pi}e^{i\psi}$. Assume that $f_\xi\ge 0$ and that there exists $x_\xi\in(0,2)$ such that $f_\xi(x_\xi)=0$. Then, as $f_\xi$ is a polynomial on $(0,2)$, we also have $f'_\xi(x_\xi)=0$ that is

$$\begin{cases} \varphi(x_\xi)+2\frac{\cos 2\psi}{\rho^2}\varphi''(x_\xi)+\frac{1}{\rho^4}\varphi^{(4)}(x_\xi) &= 0,\\ \varphi'(x_\xi)+2\frac{\cos 2\psi}{\rho^2}\varphi^{(3)}(x_\xi)+\frac{1}{\rho^4}\varphi^{(5)}(x_\xi) &= 0. \end{cases} \tag{7}$$

A computer plot shows that $\varphi''\varphi^{(5)}-\varphi^{(3)}\varphi^{(4)}\neq 0$ on $[0,2)$ so that, taking the appropriate linear combination of both equations, we get

$$2\frac{\cos 2\psi}{\rho^2}=\frac{\varphi'(x_\xi)\varphi^{(4)}(x_\xi)-\varphi(x_\xi)\varphi^{(5)}(x_\xi)}{\varphi''(x_\xi)\varphi^{(5)}(x_\xi)-\varphi^{(3)}(x_\xi)\varphi^{(4)}(x_\xi)}$$

and

$$\frac{1}{\rho^4}=\frac{\varphi'(x_\xi)\varphi''(x_\xi)-\varphi(x_\xi)\varphi^{(3)}(x_\xi)}{\varphi^{(4)}(x_\xi)\varphi^{(3)}(x_\xi)-\varphi^{(5)}(x_\xi)\varphi''(x_\xi)}.$$

In particular, $\rho$ and $\psi$ are uniquely determined by the point where $f_\xi$ and its derivative vanish.

Let us now write $f_\zeta=g+h$ with $g,h$ positive positive definite (either $L^2$ or continuous). Then, from Theorem 3.2, $g$ and $h$ have at most 4 complex zeroes and, from the proof of that theorem and the remark following it, we know that $g=\lambda f_\xi$ for some $\xi=\rho e^{i\psi}\in\mathbb{C}$ and $\lambda>0$. But $0\le g=\lambda f_\xi\le f_\zeta$ implies that $g$ must also have a double zero at $x_\zeta$. Hence, by the previous argument, we must have $\xi=\zeta$, and $g=\lambda f$. □

## 4 Hermite Functions

In this section we restrict our attention to the one-dimensional situation.

### 4.1 Preliminaries

Hermite functions are functions of the form $P(x)e^{-\lambda x^2}$ with $P$ a polynomial and $\lambda>0$. They satisfy many enjoyable properties, in particular, they provide the optimum in many *uncertainty principles*, that is, their time-frequency localization is optimal (see e.g. [21, 31] and the references therein).

Let us define the *Hermite basis functions* by

$$h_k(x)=\frac{2^{1/4}}{\sqrt{k!(4\pi)^k}}e^{\pi x^2}\partial^k e^{-2\pi x^2},\quad k=0,1,2,\dots.$$

It is well-known that $(h_k)_{k=0,1,\dots}$ form an orthonormal basis of $L^2(\mathbb{R})$, and $h_k(x)=c_kH_k(x)e^{-\pi x^2}$ with $H_k$ a real polynomial of degree $k$ with highest order term $(2\sqrt{\pi}x)^k$ and $c_k$ a normalization constant that is not relevant here. A simple computation shows that

$$H_0(x)=1,\qquad H_2(x)=4\pi x^2-1\quad\text{and}\quad H_4(x)=(4\pi x^2)^2-6(4\pi x^2)+3. \tag{8}$$

Finally, let us recall that the Hermite basis functions are eigenvectors of the Fourier transform: $\widehat{h_k} = (-i)^k h_k$. It immediately results that if the Hermite function $H(x) = P(x)e^{-\pi x^2}$ is positive positive definite, then the degree of $P$ is a multiple of 4. Indeed, $H$ has to be even, so that $P$ is real even. Then, if we expand $H$ in the Hermite basis, we get that $H(x) = \sum_{j=0}^{k} \alpha_j H_{2j}(x)e^{-\pi x^2}$ where the $\alpha_j$'s are real and $\alpha_k \neq 0$. The Fourier transform of $H$ is then given by $\widehat{H}(\xi) = \sum_{j=0}^{k}(-1)^j \alpha_j H_{2j}(\xi)e^{-\pi\xi^2}$. But, the highest order terms of the polynomial factor of $H$ and $\widehat{H}$ are then respectively $\alpha_k(4\pi x^2)^k$ and $(-1)^k\alpha_k(4\pi\xi^2)^k$. Checking that $H$ and $\widehat{H}$ stay non-negative when $x$ and $\xi$ go to infinity suffices to see that $k$ is even.

## 4.2 Gaussians Are Extremals

Let us now turn to properties of extremals among Hermite functions. The first result is a simple consequence of Hardy's Uncertainty Principle.

**Proposition 4.1** *Let $\lambda > 0$ and $P$ be a polynomial of degree $N$. Assume that $f(x) = P(x)e^{-\lambda\pi x^2}$ is a positive positive definite Hermite function. Then*

$$I(f) \subset \{Q(x)e^{-\lambda\pi x^2},\ Q \text{ a polynomial of degree } \leq N\}.$$

*In particular, if $f(x) = e^{-\lambda\pi x^2}$, then $f$ is an extremal ray generator in $\Omega^+$.*

The second part of this proposition (and its proof) seems well-known, see [10]. The proof given here is only a slight improvement.

*Proof* The second part of the proposition immediately follows from the first one.

Let $P$ be a polynomial of degree $N$ such that $f(x) = P(x)e^{-\lambda\pi x^2} \in \Omega^+$ and assume that $P(x)e^{-\lambda\pi x^2} = g(x) + h(x)$ with $g, h \in \Omega^+$. Then, as $h(x) \geq 0$, $0 \leq g(x) \leq P(x)e^{-\lambda\pi x^2}$. Further there exists a polynomial $\tilde{P}$ of degree $N$ such that $\tilde{P}(\xi)e^{-\pi\xi^2/\lambda} = \widehat{f}(\xi) = \widehat{g}(\xi) + \widehat{h}(\xi)$ so that, as $\widehat{h} \geq 0$, $0 \leq \widehat{g}(\xi) \leq \tilde{P}(\xi)e^{-\pi\xi^2/\lambda}$.

In particular, there exists a constant $C$ such that $|g(x)| \leq C(1+|x|)^N e^{-\lambda\pi x^2}$ and $|\widehat{g}(\xi)| \leq C(1+|\xi|)^N e^{-\pi\xi^2/\lambda}$. From Hardy's Uncertainty Principle ([30] see e.g. [21, 31] and [11, 17, 18] for generalizations), there exists a polynomial $Q$ of degree at most $N$ such that $g(x) = Q(x)e^{-\lambda\pi x^2}$ and therefore $h(x) = (P-Q)(x)e^{-\lambda\pi x^2}$. □

Let us conclude with the following lemma:

**Lemma 4.2** *Let $\lambda > 0$ and $P$ be a polynomial of degree $4N \geq 4$ and assume that $f(x) = P(x)e^{-\pi\lambda x^2}$ is a positive positive definite Hermite function. Write $\widehat{f}(\xi) = \widetilde{P}(\xi)e^{-\pi\xi^2/\lambda}$.*

- *If $f$ is an extremal ray generator, then either $P$ or $\widetilde{P}$ has at least 4 real zeroes.*
- *If $P$ or $\widetilde{P}$ has $4N$ real zeroes, then $f$ is an extremal ray generator.*

*Proof* It is enough to prove the lemma with $\lambda = 1$. Assume that $P$ and $\widetilde{P}$ are non-negative and have no zeroes, then there exists a constant $C > 0$ such that, $P(x) - C$ and $\widetilde{P}(\xi) - C$ are still non-negative. It follows that $\frac{P(x)-C}{2}e^{-\pi x^2}$ and its Fourier transform, $\frac{\widetilde{P}(\xi)-C}{2}e^{-\pi\xi^2}$ are both positive. As $f(x) = \frac{P(x)-C}{2}e^{-\pi x^2} + \frac{P(x)+C}{2}e^{-\pi x^2}$ we conclude that $f$ is not an extremal ray generator. It follows that $P$ or $\widetilde{P}$ has at least one zero on the real line. As they are positive polynomials, any real zero must have even multiplicity. As these polynomials are even and non-zero at the origin, we get that $P$ or $\widetilde{P}$ indeed has at least 4 real zeroes.

For the second part, it is enough to consider the case when $P$ has $4N$ real zeroes. If $f = g + h$ with $g, h \in I(f)$ then, from Proposition 4.1, we get that $g(x) = Q(x)e^{-\pi x^2}$ and $h(x) = R(x)e^{-\pi x^2}$ with $Q, R$ polynomials of degree at most $4N$. As $h \geq 0$, $0 \leq g \leq f$ thus $0 \leq Q \leq P$. It follows that a real zero of $P$ is also a real zero of $Q$. As $Q$ has not higher degree than $P$, $Q = cP$ with $0 \leq c \leq 1$ and then $g = cf$, $h = (1-c)f$. □

### 4.3 Extremal Ray Generators among Hermite Functions of Higher Degree

From the previous section, we know that if a Hermite function $f(x) = P(x)e^{-\pi x^2}$ is positive positive definite then the polynomial has degree a multiple of 4. Moreover, the interval generated by $f$ consists of Hermite functions of not higher degree. Thus, if there exists a polynomial $P$ of degree $4q$ such that $P(x)e^{-\pi x^2}$ is positive positive definite, then there exist extremals of the same degree. Indeed, we just have to consider the finite dimensional cone of positive positive definite Hermite functions of degree $4q$, which is then non-empty, and is thus the positive span of its extremal rays.

We will now characterize all positive positive definite Hermite functions of degree 4 and the extremals among them. It is enough to consider $f$ of the form $f(x) = (H_0(x) + 2aH_2(x) + bH_4(x))e^{-\pi x^2}$. Using the fact that the Hermite basis consists of eigenvalues of the Fourier transform, we get that $\widehat{f}(\xi) = (H_0(\xi) - 2aH_2(\xi) + bH_4(\xi))e^{-\pi\xi^2}$.

We thus aim at characterizing $a, b$ for which $P(x) = H_0(x) + 2aH_2(x) + bH_4(x) \geq 0$. But $H_0(x) + 2aH_2(x) + bH_4(x) = 1 + 2a + 3b - 8\pi(a+3b)x^2 + 16b\pi^2x^4$. Setting $X = 4\pi x^2$, we thus ask whether $\widetilde{P}(X) := 1 + 2a + 3b - 2(a+3b)X + bX^2 \geq 0$ for all $X \geq 0$.

The first condition is that $\widetilde{P}(0) \geq 0$ that is $1 + 2a + 3b \geq 0$ and that $\lim_{X\to+\infty} \widetilde{P}(X) \geq 0$, that is $b \geq 0$. Next, we want that $\widetilde{P}$ has no single root in $]0, +\infty)$. Thus, either $a + 3b \leq 0$ or $(a+3b)^2 - b(1 + 2a + 3b) \leq 0$ which we may rewrite as

$$(a+2b)^2 + 2\left(b - \frac{1}{4}\right)^2 \leq \frac{1}{8}. \tag{9}$$

This is the equation of an ellipse $\mathcal{E}_+$, which passes through the point $(0,0)$ where it is tangent to the line of equation $b = 0$ and through the point $(-1, 1/3)$ where it is tangent to the line of equation $1 + 2a + 3b = 0$.

In this form, we see that the set $\mathcal{D}_+$ of all $(a,b)$'s for which $P \geq 0$ is the union of the ellipse of (9) and the triangle formed by the lines $b = 0$, $a + 3b = 0$ and $1 + 2a + 3b = 0$, that is the triangle with vertices $(0,0)$, $(-1, 1/3)$ $(-1/2, 0)$.

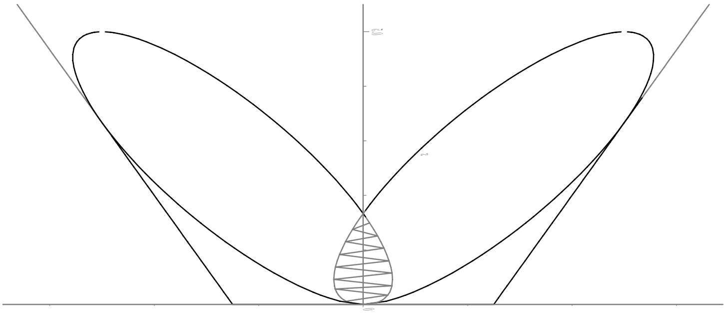

**Fig. 1** The set of all $(a, b)$'s for which $f_{a,b}$ is positive positive definite

If we want $f$ to be positive positive definite, then both $(a, b)$ and $(-a, b)$ have to belong to $\mathcal{D}_+$. It is easy to see that this reduces to the intersection of the two ellipses. More precisely we get:

**Proposition 4.3** *The set of all Hermite functions of order* 4 *that are positive positive definite is given by* $f_{a,b} := (H_0 + 2aH_2 + bH_4)e^{-\pi x^2}$ *where* $(a, b)$ *belongs to the region* $\mathcal{D}$ *represented in Fig.* 1 *and parametrized by the following*:

- *either* $a \geq 0$ *and* $(a + 2b)^2 + 2(b - 1/4)^2 \leq 1/8$;
- *or* $a \leq 0$ *and* $(-a + 2b)^2 + 2(b - 1/4)^2 \leq 1/8$.

Moreover $f_{a,b}$ is an extremal ray generator of $\Omega^+$ if and only if $(a, b) \in \partial\mathcal{D}$, where $\partial\mathcal{D}$ is the boundary of $\mathcal{D}$.

The last part results directly from the fact that $\mathcal{D}$ is convex and that all its boundary points are points of curvature (excepted two) and are thus extreme points of $\mathcal{D}$. The fact that $f_{a,b}$ is then an extremal of $\Omega^+$ is a direct consequence of the previous discussion.

It should also be noted that if $f_{a,b}$ is an extremal ray generator, then

- either $f_{a,b}$ has only real zeroes and $\widehat{f_{a,b}}$ is positive, in which case we will say that $f_{a,b}$ is of the *time type*;
- or $\widehat{f_{a,b}}$ has only real zeroes and $f_{a,b}$ is positive, in which case we will say that $f_{a,b}$ is of the *frequency type*.

**Corollary 4.4** *Assume that* $f_{a_1,b_1}, \ldots, f_{a_N,b_N}$ *are all of the time type, then* $f = \prod_{i=1}^N f_{a_i,b_i}$ *is an extreme ray generator in* $\mathcal{C}$.

*If* $f_{a_1,b_1}, \ldots, f_{a_N,b_N}$ *are all of the frequency type, then* $f = \star_{i=1}^N f_{a_i,b_i}$ *is an extreme ray generator in* $\mathcal{C}$.

*Proof* Let us first assume that all the $f_{a_i,b_i}$'s are of time type and consider $f = \prod_{i=1}^N f_{a_i,b_i}$. If this is extremal, then $\widehat{f} = \star_{i=1}^N f_{-a_i,b_i}$ is also extremal.

Let us write $f = P\gamma^N = g + h$ with $P$ a polynomial, $\gamma$ the standard Gaussian, $g, h \in \Omega^+$. From Proposition 4.1, we know that both $g$ and $h$ are Hermite functions, $g = G\gamma^N$ and $h = H\gamma^N$ with $G$, $H$ positive polynomials of degree $\leq 4N$.

But, as $h \geq 0$, $0 \leq G \leq P$ and every real zero of $P$ is thus a real zero of $G$. As $P$ is assumed to have $4N$ real zeroes, $G$ has $4N$ real zeroes. As $G$ is of degree at most $4N$, $G = \lambda P$ thus $g = \lambda f$ and $h = (1-\lambda) f$.

If all the $f_{a_i,b_i}$'s are of frequency type, the same argument applies on the Fourier side. □

## 5 Some Important Classes of Positive Positive Definite Functions

In this section, we will show that several criteria available in the literature are particular cases of Choquet representation of the cone $\Omega_d^+$. We will appeal several times to Lemma 2.1.

### 5.1 Non-Negative Convex Functions

A well-known class of positive definite functions is that of *Pólya type* functions (see [40]). More precisely, $f$ is said to be of Pólya type if $f$ is even, continuous, convex on $[0,+\infty)$ and $f(x) \to 0$ when $x \to \infty$. It is well-known that $f$ is of Pólya type if and only if there exists a positive bounded measure $\nu$ on $[0,+\infty)$ such that, for all $x \in \mathbb{R}$

$$f(x) = \int_0^{+\infty} (1 - |x|/t)_+ \, \mathrm{d}\nu(t). \tag{10}$$

Note that Lebesgue's theorem ensures that a function $f$ given by (10) is continuous as soon as the measure $\nu$ appearing in that formula is bounded.

Further, one may show that if $f$ is a Pólya function then $f$ is a Fourier transform of a measure of the form $p(\xi)\,\mathrm{d}\xi$ with $p$ continuous on $\mathbb{R} \setminus \{0\}$. More precisely, $\nu$ and $p$ are related by

$$p(\xi) = c \int_0^{+\infty} \left( \frac{\sin(\pi t \xi)}{t\xi} \right)^2 t \, \mathrm{d}\nu(t)$$

where $c$ is some constant (and $\frac{\sin 0}{0} = 1$).

Note that everything is straightforward when $f$ has sufficient smoothness and decay, using integrations by part. For a simple proof in the general case and further references, we refer to [42].

Finally, an easy computation shows that $(1-|x|/t)_+ = c\chi_{[-t/2,t/2]} * \chi_{[-t/2,t/2]}(x)$ which is an extremal ray generator according to Theorem 3.2. We may thus rewrite (10) in the form

$$f(x) = \int_0^{+\infty} \chi_{[-t/2,t/2]} * \chi_{[-t/2,t/2]}(x) \, \mathrm{d}\nu(t). \tag{11}$$

In this form, we immediately see that we are in the situation of Lemma 2.1.

**Proposition 5.1** *Let $f$ be a Pólya type function. Then $f$ is positive positive definite, and it is an extremal ray generator if and only if $f = \chi_{[-r/2,r/2]} * \chi_{[-r/2,r/2]}$ for some $r > 0$.*

*Example*

- $\psi(t) = \frac{\ln(e+|t|)}{1+|t|}$ and $\psi(t) = \frac{1}{(1+|t|)^\alpha}$, $\alpha > 0$ are of Pólya type and are thus not extremal ray generators.
- It is easy to show that $e^{-|x|^p}$ is of Pólya type for $0 < p \leq 1$, in particular, they are not extremal ray generators. We will show below that this stays true for $1 < p < 2$ as well.

### 5.2 Generalizations by Gneiting

Pólya's criterion has been extended recently by Gneiting [24, 25] and by C. Hainzl and R. Seiringer [29]. For instance, [24] characterizes those functions which can be written in the form

$$\psi(x) = \int_0^{+\infty} w(xt)\,\mathrm{d}\mu(t) \tag{12}$$

where $w(x) := (1-x^2)_+ * (1-x^2)_+$ and $\mu$ is a positive bounded measure on $[0,+\infty)$. Note that $w$ is the positive positive definite function introduced by Wu in the study of radial basis function interpolation and that $w(x) = c(1-|x|)_+^3(1 + 3/2|x| + x^2/4)$ where $c$ is a constant. This function also plays an important role in the work of Wendland [49] on positive definite functions with compact support of optimal smoothness.

More precisely, Gneiting showed that a function $\psi(t) = \varphi(|t|)$ can be written in the form (12) if and only if $\varphi$ satisfies

(i) $\varphi$ is twice continuously differentiable,
(ii) $\varphi(0) > 0$ and $\varphi(x) \to 0$ when $x \to +\infty$,
(iii) $\frac{1}{t}(\sqrt{t}\varphi''(\sqrt{t}) - \varphi'(\sqrt{t}))$ is convex.

Note that such a function is necessarily non-negative.

The same proof as in the previous section then shows the following:

**Proposition 5.2** *A function $\psi$ of the form* (12) (*or equivalently a function $\psi$ given by $\psi(t) = \varphi(|t|)$ with $\varphi$ satisfying* (i)–(iii) *above*) *is positive positive definite*, *and it is an extremal ray generator in the set of positive positive definite functions if and only if there exists $c > 0$ such that $\psi(t) = w(ct)$.*

*Example* As already noted by Gneiting, the following functions satisfy (12) and are therefore not extremal ray generators:

$$\begin{aligned}
&\text{(i)} && \psi(t) = \frac{1}{1+|t|^\beta}, \quad 0 < \beta < 1.877\ldots,\\
&\text{(ii)} && \psi(t) = (1+\gamma|t|+t^2)\exp(-|t|), \quad 0 < \gamma < 1/4,\\
&\text{(iii)} && \psi(t) = (1-|t|)_+^3(1+3|t|),\\
&\text{(iv)} && \psi(t) = (1-|t|^\lambda)_+^3.
\end{aligned}$$

The first one is known as Linnik's function and is of Pólya type for $\beta < 1$. The third one has been introduced by Wendland and has interesting optimal smoothness properties. The last one is called Kuttner's function and seems to be Gneiting's original motivation in the above characterization.

Finally, $\psi(t) = \exp(-|t|^\beta)$ satisfies the hypothesis of the theorem for $\beta < 1.84170$ thus improving the domain of non-extremality found in the previous section.

### 5.3 Bernstein Functions

Let us recall that a non-negative function $g$ on $[0, +\infty)$ is called *completely monotonic* if it is infinitely differentiable on $(0, +\infty)$ and, for all $k \in \mathbb{N}$ and $x \in (0, +\infty)$,

$$(-1)^k g^{(k)}(x) \geq 0.$$

Completely monotonic functions have remarkable applications in different branches. For instance, they play a role in potential theory [5], probability theory [9, 19, 33], physics [16], numerical and asymptotic analysis [22, 51], and combinatorics [2]. A detailed collection of the most important properties of completely monotonic functions can be found in [50, Chap. IV], and in an abstract setting in [6].

The celebrated theorem of Bernstein (see [4, Chap. III, Sect. 2], [19, Chap. 18, Sect. 4] or [50, p. 161]) states that every completely monotonic function which is continuous at zero is the Laplace transform of a positive bounded measure on $[0, +\infty)$. In other words, $g$ is completely monotonic and continuous at 0 if and only if there exists a (necessarily unique) positive bounded measure $\mu$ on $[0, +\infty)$ such that, for every $x \geq 0$,

$$g(x) = \int_0^{+\infty} e^{-tx} \, \mathrm{d}\mu(t). \tag{13}$$

A particular case of Lemma 2.1, of which the first part is well-known, is then the following:

**Proposition 5.3** *Let $g$ be a non-negative, completely monotonic function, continuous at* 0. *Let $f$ be defined on $\mathbb{R}^d$ by $f(x) = g(|x|^2)$. Then $f$ is a positive positive definite function and is an extremal ray generator if and only if $f$ is a Gaussian.*

*Example*

- Let $\lambda > 0$ and $0 < \alpha \leq 1$. It is well-known and easy to show that $g$ defined by $g(t) = e^{-\lambda t^\alpha}$ is completely monotonic. It follows that $e^{-\lambda |x|^p}$ is positive positive definite for $0 < p \leq 2$ and an extremal ray generator only for $p = 2$.
- Let $\alpha \neq 0$ and $\beta > 0$. It is easy to show that $g(t) = (t + \alpha^2)^{-\beta}$ (the so-called *inverse multiquadrics*) is completely monotonic. It follows that $(x^2 + \alpha^2)^{-\beta}$ is positive positive definite but not an extremal ray generator.
- Recently, the so-called Dagum family $D_{\beta,\gamma}(x) = 1 - (\frac{x^\beta}{1+x^\beta})^\gamma$ has been introduced in [38, 41] where it was shown that the Dagum class allows for treating independently the fractal dimension and the Hurst effect of the associated weakly stationary Gaussian RF, by using the procedure suggested in [26]. In [7], the authors further showed that for certain parameters, this function is completely monotonic.

Note that completely monotonic functions allow to construct radial positive definite functions in *any* dimension. There is a converse to this. More precisely, let $f_0$ be a continuous function on $[0, +\infty)$ and define $f_d$ on $\mathbb{R}^d$ by $f_d(x) = f_0(|x|)$. Observe that if $f_d$ is positive definite then $f_{d'}$ is also positive definite for any $d' < d$. A famous theorem of Schoenberg [43] (see also [45] for a more modern proof and further references or [3] for another proof) states that if $f_d$ is positive definite for any $d$, then $f_0(x) = g(x^2)$ with $g$ completely monotonic.

## 6 Conclusion

In this paper we have investigated the extremal ray generators of the cone of continuous positive positive definite functions for which we have described two important classes of such extremals.

At this stage, we would first like to stress that, up to minor modifications, most of our results stay true for positive positive definite $L^2$ functions or even tempered distributions. Let us recall that in this case, one can not define positive definiteness via (14). One thus replaces this condition by one that is equivalent for continuous functions. To do so, notice that if $f$ is continuous, then $f$ is positive definite if and only if, for every smooth function $\Phi \in \mathcal{S}(\mathbb{R}^d)$ in the Schwartz-class,

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(x-y)\Phi(x)\overline{\Phi(y)}\,\mathrm{d}x\,\mathrm{d}y \geq 0. \tag{14}$$

Note that this makes sense if $f$ is only assumed to be in $L^\infty$, but in that case it is well-known (e.g. [4, 14, 39]) that implies that $f$ is almost everywhere equal to a continuous function. Further, we may extend (14) to $T \in \mathcal{S}'$ and take this to be the definition of a positive definite tempered distribution: a tempered distribution $T$ is positive definite if for every $\Phi \in \mathcal{S}(\mathbb{R}^d)$, $\langle T, \Phi * \Phi^* \rangle \geq 0$ where $\Phi^*(x) = \overline{\Phi(-x)}$. Schwartz [44] extended Bochner's theorem by characterizing positive definite tempered distributions as the Fourier transforms of positive tempered measures, that is $\langle T, \Phi \rangle = \int_{\mathbb{R}^d} \widehat{\Phi}(\xi)\,\mathrm{d}\mu(\xi)$ where $\mu$ is a positive measure such that, for some $\alpha > 0$, $\int_{\mathbb{R}^d}(1 + |\xi^2|)^{-\alpha}\,\mathrm{d}\mu(\xi) < +\infty$. A proof based on Choquet Theory may be found in [47]. As a particular case, one gets that if $T \in L^2$, then $T$ is positive definite if and only if $\widehat{T} \geq 0$. For further extensions of the notion of positive definiteness, we refer to [46].

Unfortunately, several open problems remain, but some features seem to have become clear:

- A full classification of the extremals is probably impossible and no reasonable conjecture can be stated at this stage. For instance, the existence of an extremal compactly supported function with Fourier transform having complex zeroes leaves little hope for a full description of compactly supported extremals. As for the extremals inside the Hermite class, we have a full description only up to degree 4. For higher degree, even though we have been able to construct extremals, we are far from a full description. The main reason for this, is that we are unable to decide the answer of the following question:

**Question 1**

(a) *Is the product of two extremals an extremal?*
(b) *What about the convolution of two extremals* (*if it makes sense*)*?*

We have no hint of what the answer might be and will therefore not propose a conjecture.

– There are many criteria allowing to decide whether a function is positive definite. As we have seen, these criteria actually characterize the functions that are mixtures of the scales of a single extremal inside the class of positive positive definite functions. We are thus tempted to ask for more criteria, for instance:

**Question 2**

(a) *Find a criterion that allows to decide whether a function is the mixture of the scales of* $m_\alpha * m_\alpha$, *where* $\alpha$ *may, or may not be fixed.*
(b) *Find a criterion that allows to decide whether a function is the mixture of extremals of scales of extremal Hermite functions of order* 4.
(c) *Find a criterion for positive definiteness that is not given in terms of a mixture of positive positive definite functions*, *thus also characterizing positive definite functions that are not necessarily non-negative.*

– Finally, all the extremals we found, except the Gaussians, either have at least a zero, or their Fourier transform has at least a zero. Borisov [10] conjectured that the only extremals in $L^2(\mathbb{R}) \cap \mathcal{C}(\mathbb{R})$ that are strictly positive and that have strictly positive Fourier transform are the Gaussian functions $e^{-a\pi x^2}$, $a > 0$. We are inclined to believe that this is false. This is linked to Question 1 above which leads us to the following more precise question:

**Question 3** *Consider the two functions* $f = \chi_{[-1/2,1/2]} * \chi_{[-1/2,1/2]}$ *and* $\gamma = e^{-\pi x^2}$, *and recall that they are extremal positive positive definite functions in* $\Omega_1^+$. *Is* $f * \gamma$ *extremal in* $\Omega_1^+$ *and, if so, is* $\gamma(f * \gamma)$ *extremal in* $\Omega_1^+$*?*

A positive answer to the second question would of course provide a counterexample to Borisov's conjecture.

Overall, we hope this paper will help reviving P. Levy's request to study the cone of positive positive definite functions.

## References


1. Akemann, C.A., Walter, M.E.: Non-Abelian Pontriagin duality. Duke Math. J. **39**, 17–38 (1972)
2. Ball, K.: Completely monotonic rational functions and Hall's marriage theorem. J. Comb. Theory, Ser. B **61**, 118–124 (1994)
3. Baxter, B.J.C.: Positive definite functions on Hilbert space. East J. Approx. **10**, 269–274 (2004)
4. Becker, R.: Convex Cones in Analysis. Travaux en cours, vol. 67. Hermann, Paris (2006)
5. Berg, C., Forst, G.: Potential Theory on Locally Compact Abelian Groups. Ergebnisse der Math., vol. 87. Springer, Berlin (1975)

6. Berg, C., Christensen, J.P.R., Ressel, P.: Harmonic Analysis on Semigroups. Theory of Positive Definite and Related Functions. Graduate Texts in Mathematics, vol. 100. Springer, Berlin (1984)
7. Berg, C., Mateu, J., Porcu, E.: The Dagum family of isotropic correlation functions. Available at arXiv:0705.0456v1 [math.ST]
8. Bochner, S.: Monotone Funktionen, Stieltjessche Integrale und harmonische Analyse. Math. Ann. **108**, 378–410 (1933)
9. Bondesson, L.: Generalized Gamma Convolutions and Related Classes of Distributions and Densities. Lecture Notes in Statistics, vol. 76. Springer, New York (1992)
10. Borisov, A.: Positive positive definite functions on Abelian groups. Preprint (1999). Available on arXiv:math/9906126v1
11. Bonami, A., Demange, B., Jaming, Ph.: Hermite functions and uncertainty principles for the Fourier and the windowed Fourier transforms. Rev. Mat. Iberoam. **19**, 23–55 (2003)
12. Bucy, R.S., Maletese, G.: Extreme positive definite functions and Choquet's representation theorem. J. Math. Anal. Appl. **12**, 371–377 (1965)
13. Buhmann, M.D.: Radial Basis Functions: Theory and Implementations. Cambridge Monographs on Applied and Computational Mathematics, vol. 12. Cambridge University Press, Cambridge (2003)
14. Choquet, G.: Deux exemples classiques de représentation intégrale. Enseign. Math. **15**, 63–75 (1969)
15. Choquet, G.: Lectures on Analysis. Benjamin, Elmsford (1969). Marsen, J., Lance, T., Gelbart, S. (eds.)
16. Day, W.A.: On monotonicity of the relaxation functions of viscoelastic material. Proc. Camb. Philos. Soc. **67**, 503–508 (1970)
17. Demange, B.: Principes d'incertitude associés à des formes quadratiques non dégénérées. Thèse de l'université d'Orléans (2004)
18. Demange, B.: Uncertainty principles related to quadratic forms. Mem. Soc. Math. Fr. (2009, to appear)
19. Feller, W.: An Introduction to Probability Theory and Applications. Willey, New York (1971)
20. Folland, G.B.: A Course in Abstract Harmonic Analysis. Studies in Advanced Mathematics. CRC Press, Boca Raton (1995)
21. Folland, G.B., Sitaram, A.: The uncertainty principle: a mathematical survey. J. Fourier Anal. Appl. **3**, 207–238 (1997)
22. Frenzen, C.L.: Error bounds for asymptotic expansions of the ratio of two gamma functions. SIAM J. Math. Anal. **18**, 890–896 (1987)
23. Giraud, B.G., Peschanski, R.: On positive functions with positive Fourier transforms. Acta Phys. Pol. B **37**, 331–346 (2006)
24. Gneiting, T.: Kuttner's problem and a Pólya type criterion for characteristic functions. Proc. Am. Math. Soc. **128**, 1721–1728 (2000)
25. Gneiting, T.: Criteria of Pólya type for radial positive definite functions. Proc. Am. Math. Soc. **129**, 2309–2318 (2001)
26. Gneiting, T., Schlather, M.: Stochastic models that separate fractal dimension and the Hurst effect. SIAM Rev. **46**, 269–282 (2004)
27. Godefroy, G.: Personal communication
28. Grafakos, L.: Classical and Modern Fourier Analysis. Prentice Hall, New York (2004)
29. Hainzl, C., Seiringer, R.: General decomposition of radial functions on $\mathbb{R}^n$ and applications to $N$-body quantum systems. Lett. Math. Phys. **61**, 75–84 (2002)
30. Hardy, G.H.: A theorem concerning Fourier transforms. J. Lond. Math. Soc. **8**, 227–231 (1933)
31. Havin, V., Jöricke, B.: The Uncertainty Principle in Harmonic Analysis. Springer, Berlin (1994)
32. Hurwitz, A.: Über die Nullstellen der Bessel'schen Funktion. Math. Ann. **33**, 246–266 (1889). See Mathematische Werke **1**, 266–286 (1932)
33. Kimberling, C.H.: A probabilistic interpretation of complete monotonicity. Aequ. Math. **10**, 152–164 (1974)
34. Kaniuth, E., Lau, A.T.: A separation property of positive definite functions on locally compact groups and applications to Fourier algebras. J. Funct. Anal. **175**, 89–110 (2000)
35. Kaniuth, E., Lau, A.T.: Extension and separation properties of the positive definite functions on locally compact groups. Trans. Am. Math. Soc. **359**, 447–463 (2007)
36. Koldobsky, A.: Fourier Analysis in Convex Geometry. Mathematical Surveys and Monographs, vol. 116. Am. Math. Soc., Providence (2005)
37. Lévy, P.: Fonctions caractéristiques positives (Positive characteristic functions). C.R. Acad. Sci. Paris, Sér. A–B **265**, 249–252 (1967)

38. Mateu, J., Porcu, E., Nicolis, O.: A note on decoupling of local and global behaviour for the Dagum random field. Probab. Eng. Mech. **28**, 320–329 (2007)
39. Phelps, R.: Lectures on Choquet's Theorem. Van Nostrand, Princeton (1966)
40. Pólya, G.: Remarks on characteristic functions. In: Neyman, J. (ed.) Proceedings of the Berkeley Symposium on Mathematical Statistics and Probability, pp. 115–123. University of California Press, Berkeley (1949)
41. Porcu, E., Mateu, J., Zini, A., Pini, R.: Modelling spatiotemporal data: a new variogram and covariance structure proposal. Stat. Probab. Lett. **77**, 83–89 (2007)
42. Sasvári, Z.: On a classical theorem in the theory of Fourier integrals. Proc. Am. Math. Soc. **126**, 711–713 (1998)
43. Schoenberg, I.J.: Metric spaces and completely monotone functions. Ann. Math. **39**, 811–841 (1938)
44. Schwartz, L.: Théorie des distributions. Vol. II. Actualités Sci. Indust., vol. 1122. Hermann, Paris (1951)
45. Steerneman, A.G.M., van Perlo-ten Kleij, F.: Spherical distributions: Schoenberg (1938) revisited. Exp. Math. **23**, 281–287 (2005)
46. Steward, J.: Positive definite functions and generalizations, an historical survey. Rocky Mt. J. Math. **6**, 409–434 (1976)
47. Thomas, E.G.F.: Bochner and Bernstein theorems via the nuclear integral representation theorem. Special issue dedicated to John Horváth. J. Math. Anal. Appl. **297**, 612–624 (2004)
48. Watson, G.N.: A Treatise on the Theory of Bessel Functions, 2nd edn. Cambridge University Press, Cambridge (1944)
49. Wendland, H.: Piecewise polynomial, positive definite and compactly supported radial functions of minimal degree. J. Convex Anal. **4**, 389–396 (1995)
50. Widder, D.V.: The Laplace Transform. Princeton Univ. Press, Princeton (1941)
51. Wimp, J.: Sequence Transformations and Their Applications. Academic Press, San Deigo (1981)
52. Wu, Z.: Compactly supported positive definite radial functions. Adv. Comput. Math. **4**, 283–292 (1995)