Characterization and construction of radial basis functions

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Abstract

We review characterizations of (conditional) positive definiteness and show how they apply to the theory of radial basis functions. We then give complete proofs for the (conditional) positive definiteness of all practically relevant basis functions. Furthermore, we show how some of these characterizations may lead to construction tools for positive definite functions. Finally, we give new construction techniques based on discrete methods which lead to non-radial, even non-translation invariant, local basis functions.

1 Introduction

Radial basis functions are an efficient tool for solving multivariate scattered data interpolation problems. To interpolate an unknown function $f \in C(\Omega)$ whose values on a set $X = \{x_1, \ldots, x_N\} \subset \Omega \subset I\!R^d$ are known, a function of the form

$$s_{f,X}(x) = \sum_{j=1}^{N} \alpha_j \Phi(x, x_j) + p(x) \qquad (1)$$

is chosen, where p is a low degree polynomial and $\Phi : \Omega \times \Omega \to I\!R$ is a fixed function. The numerical treatment can be simplified in the special situations

1. $\Phi(x, y) = \phi(x - y)$ with $\phi : I\!R^d \to I\!R$ (*translation invariance*),
2. $\Phi(x, y) = \phi(\|x - y\|_2)$ with $\phi : [0, \infty) \to I\!R$ (*radiality*),

and this is how the notion of *radial basis functions* arose. The most prominent examples of radial basis functions are:

$$\phi(r) \;=\; r^\beta, \quad \beta > 0, \quad \beta \notin 2I\!N,$$

$$
\begin{aligned}
\phi(r) &= r^{2k}\log(r), \quad k \in I\!N \quad \text{(thin-plate splines)},\\
\phi(r) &= (c^2+r^2)^\beta, \quad \beta < 0, \quad \text{(inverse multiquadrics)}\\
\phi(r) &= (c^2+r^2)^\beta, \quad \beta > 0, \quad \beta \notin I\!N \quad \text{(multiquadrics)}\\
\phi(r) &= e^{-\alpha r^2}, \quad \alpha > 0 \quad \text{(Gaussians)},\\
\phi(r) &= (1-r)_+^4(1+4r).
\end{aligned}
$$

All of these basis functions can be uniformly classified using the concept of (conditionally) positive definite functions:

Definition 1.1 *A continuous function $\Phi : \Omega \times \Omega \to \mathbb{C}$ is said to be conditionally positive (semi–) definite of degree m on Ω if for all $N \in I\!N$, all distinct $x_1, \ldots, x_N \in \Omega$, and all $\alpha \in \mathbb{C}^N \setminus \{0\}$ satisfying*

$$\sum_{j=1}^{N} \alpha_j p(x_j) = 0 \tag{2}$$

for all polynomials p of degree less than m the quadratic form

$$\sum_{j=1}^{N}\sum_{k=1}^{N} \alpha_j \overline{\alpha_k} \Phi(x_j, x_k) \tag{3}$$

is positive (nonnegative). The function Φ is positive definite if it is conditionally positive definite of order $m = 0$.

Note that in case of a positive definite function the conditions (2) are empty and hence (3) has to be positive for all $\alpha \in \mathbb{C}^N \setminus \{0\}$. Finally, if Φ is a symmetric real-valued function, it is easy to see that it suffices to test only real α.

The use of this concept in the context of multivariate interpolation problems is explained in the next theorem, which also shows the connection between the degree of the polynomial p in (1) and the order m of conditional positive definiteness of the basis function Φ. We will denote the space of d-variate polynomials of degree at most m by $\pi_m(I\!R^d)$.

Theorem 1.2 *Suppose Φ is conditionally positive definite of oder m on $\Omega \subseteq I\!R^d$. Suppose further that the set of centers $X = \{x_1, \ldots, x_N\} \subseteq \Omega$ is $\pi_{m-1}(I\!R^d)$ unisolvent, i.e. the zero polynomial is the only polynomial from $\pi_{m-1}(I\!R^d)$ that vanishes on X. Then for given $f_1, \ldots, f_N$ there is exactly one function $s_{f,X}$ of the form (1) with a polynomial $p \in \pi_{m-1}(I\!R^d)$ such that $s_{f,X}(x_j) = f_j$, $1 \le j \le N$ and $\sum_{j=1}^N \alpha_j q(x_j) = 0$ for all $q \in \pi_{m-1}(I\!R^d)$.*

It is the goal of this paper to give full proofs for the conditional positive definiteness of all aforementioned radial basis functions and to use the ideas behind these proofs to construct new ones. We only rely on certain analytical tools that are not directly related to radial basis functions.

2 The Schoenberg-Micchelli Characterization

Given a continuous univariate function $\phi : [0, \infty) \to \mathbb{R}$ we can form the function $\Phi(x, y) := \phi(\|x - y\|_2)$ on $\mathbb{R}^d \times \mathbb{R}^d$ for arbitrary space dimension d. Then we can say that ϕ is conditionally positive definite of order m on $\mathbb{R}^d$, iff Φ is conditionally positive definite of order m on $\mathbb{R}^d$ in the sense of Definition 1.1.

Taking this point of view, we are immediately led to the question of whether a univariate function ϕ is conditionally positive definite of some order m on $\mathbb{R}^d$ *for all* $d \geq 1$. This question was fully answered in the positive definite case by Schoenberg [16] in 1938 in terms of completely monotone functions. In the case of conditionally positive definite functions Micchelli [12] generalized the sufficient part of Schoenberg's result, suspecting that it was also necessary. This was finally proved by Guo, Hu and Sun [9].

Definition 2.1 *A function $\phi : (0, \infty) \to \mathbb{R}$ is said to be completely monotone on $(0, \infty)$ if $\phi \in C^\infty(0, \infty)$ and*

$$(-1)^\ell \phi^{(\ell)}(r) \geq 0, \qquad \ell \in \mathbb{N}_0, \quad r > 0. \tag{4}$$

A function $\phi : [0, \infty) \to \mathbb{R}$ is said to be completely monotone on $[0, \infty)$ if it is completely monotone on $(0, \infty)$ and continuous at zero.

Theorem 2.2 *(Schoenberg) Suppose $\phi : [0, \infty) \to \mathbb{R}$ is not the constant function. Then ϕ is positive definite on every $\mathbb{R}^d$ if and only if the function $t \mapsto \phi(\sqrt{t})$, $t \in [0, \infty)$ is completely monotone on $[0, \infty)$.*

Schoenberg's characterisation of positive definite functions allows us to prove positive definiteness of Gaussians and inverse multiquadrics without difficulty:

Theorem 2.3 *The Gaussians $\phi(r) = e^{-\alpha r^2}$, $\alpha > 0$, and the inverse multiquadrics $\phi(r) = (c^2 + r^2)^\beta$, $c > 0$, $\beta < 0$, are positive definite on $\mathbb{R}^d$ for all $d \geq 1$.*

Proof: For the Gaussians note that

$$f(r) := \phi(\sqrt{r}) = e^{-\alpha r}$$

satisfies $(-1)^\ell f^{(\ell)}(r) = \alpha^\ell e^{-\alpha r} > 0$ for all $\ell \in \mathbb{N}_0$ and $\alpha, r > 0$. Similarly, for the inverse multiquadrics we find with $f(r) := \phi(\sqrt{r}) = (c^2 + r)^{-|\beta|}$ that

$$(-1)^\ell f^{(\ell)}(r) = (-1)^{2\ell} |\beta| (|\beta| + 1) \cdot \ldots \cdot (|\beta| + \ell - 1)(r + c^2)^{-|\beta| - \ell} > 0.$$

Since in both cases ϕ is not the constant function, the Gaussians and inverse multiquadrics are positive definite. $\square$

There are several other characterizations of completely monotone functions (see [19]), which by Schoenberg's theorem also apply to positive definite functions. The most important is the following one by Bernstein (see Widder [19]). It implies that the proper tool to handle positive definite functions on $\mathbb{R}^d$ for all $d \geq 1$, is the Laplace transform.

Theorem 2.4 *(Bernstein) A function ϕ is positive definite on $\mathbb{R}^d$ for all $d \geq 1$, if and only if there exists a nonzero, finite, nonnegative Borel measure μ, not supported in zero, such that ϕ is of the form*

$$\phi(r) = \int_0^\infty e^{-r^2 t} d\mu(t). \tag{5}$$

Note that the sufficient part of Bernstein's theorem is easy to prove, if we know that the Gaussians are positive definite. For every $\alpha \in \mathbb{R}^N \setminus \{0\}$ and every distinct $x_1, \ldots, x_N \in \mathbb{R}^d$ the quadratic form is given by

$$\sum_{j,k=1}^N \alpha_j \alpha_k \phi(\|x_j - x_k\|_2) = \int_0^\infty \left| \sum_{j=1}^N \alpha_j e^{-t\|x_j - x_k\|_2^2} \right|^2 d\mu(t).$$

Another consequence of this theory is the following.

Theorem 2.5 *Suppose $\phi : [0, \infty) \to \mathbb{R}$ is positive definite on $\mathbb{R}^d$ for all $d \geq 1$. Then ϕ has no zero. In particular, there exists no compactly supported univariate function that is positive definite on $\mathbb{R}^d$ for all $d \geq 1$.*

Proof: Since ϕ is positive definite on $\mathbb{R}^d$ for all $d \geq 1$, there exists a finite, nonzero, nonnegative Borel measure μ on $[0, \infty)$ such that (5) holds. If r_0 is a zero of ϕ this gives

$$0 = \int_0^\infty e^{-r_0^2 t} d\mu(t).$$

Since the measure is non-negative and the weight function $e^{-r_0^2 t}$ is positive we find that the measure must be the zero measure. $\square$

Thus the compactly supported function $\phi(r) = (1-r)_+^4(1+4r)$ given in the introduction cannot be positive definite on $\mathbb{R}^d$ for all $d \geq 1$, and it is actually only positive definite on $\mathbb{R}^d$, $d \leq 3$. If one is interested in constructing basis functions with compact support, one has to take the above negative result into account. We shall see in the next section that the Fourier transform is the right tool to handle positive definite translation–invariant functions on $I\!R^d$ with a prescribed d. But before that, let us have a look at *conditionally* positive definite functions. We will state only the sufficient part as provided by Micchelli [12].

Theorem 2.6 *(Micchelli) Given a function $\phi \in C[0,\infty)$, define $f = \phi(\sqrt{\cdot})$. If there exists an $m \in I\!N_0$ such that $(-1)^m f^{(m)}$ is well–defined and completely monotone on $(0,\infty)$, then ϕ is conditionally positive semi-definite of order m on $I\!R^d$ for all $d \geq 1$. Furthermore, if f is not a polynomial of degree at most m, then ϕ is conditionally positive definite.*

This theorem allows us to classify all functions from the introduction, with the sole exception of the compactly supported one. However, to comply with the notion of conditional positive definiteness, we shall have to adjust the signs properly. To do this we denote the smallest integer greater than or equal to x by $\lceil x \rceil$.

Theorem 2.7 *The multiquadrics $\phi(r) = (-1)^{\lceil \beta \rceil}(c^2+r^2)^\beta$, $c, \beta > 0$, $\beta \notin I\!N$, are conditionally positive definite of order $m \geq \lceil \beta \rceil$ on $I\!R^d$ for all $d \geq 1$.*

Proof: If we define $f_\beta(r) = (-1)^{\lceil \beta \rceil}(c^2 + r)^\beta$, we find

$$f_\beta^{(k)}(r) = (-1)^{\lceil \beta \rceil}\beta(\beta - 1) \cdot \ldots \cdot (\beta - k + 1)(c^2 + r)^{\beta - k},$$

which shows that $(-1)^{\lceil \beta \rceil} f_\beta^{(\lceil \beta \rceil)}(r) = \beta(\beta - 1) \cdot \ldots \cdot (\beta - \lceil \beta \rceil + 1)(c^2 + r)^{\beta - \lceil \beta \rceil}$ is completely monotone, and that $m = \lceil \beta \rceil$ is the smallest possible choice of m to make $(-1)^m f^{(m)}$ completely monotone. □

Theorem 2.8 *The functions $\phi(r) = (-1)^{\lceil \beta/2 \rceil} r^\beta$, $\beta > 0$, $\beta \notin 2I\!N$, are conditionally positive definite of order $m \geq \lceil \beta/2 \rceil$ on $I\!R^d$ for all $d \geq 1$.*

Proof: Define $f_\beta(r) = (-1)^{\lceil \frac{\beta}{2} \rceil} r^{\frac{\beta}{2}}$ to get

$$f_\beta^{(k)}(r) = (-1)^{\lceil \frac{\beta}{2} \rceil} \frac{\beta}{2}(\frac{\beta}{2} - 1) \cdots (\frac{\beta}{2} - k + 1) r^{\frac{\beta}{2} - k}.$$

This shows that $(-1)^{\lceil \frac{\beta}{2} \rceil} f_\beta^{(\lceil \frac{\beta}{2} \rceil)}(r)$ is completely monotone and $m = \lceil \frac{\beta}{2} \rceil$ is the smallest possible choice. □

Theorem 2.9 *The thin–plate or surface splines $\phi(r) = (-1)^{k+1} r^{2k} \log(r)$ are conditionally positive definite of order $m = k + 1$ on every $I\!R^d$.*

Proof: Since $2\phi(r) = (-1)^{k+1} r^{2k} \log(r^2)$ we set $f_k(r) = (-1)^{k+1} r^k \log(r)$. Then it is easy to see that

$$f_k^{(\ell)}(r) = (-1)^{k+1} k(k-1)\cdots(k-\ell+1) r^{k-\ell} \log(r) + p_\ell(r), \qquad 1 \le \ell \le k,$$

where p_ℓ is a polyonmial of degree $k-\ell$. This means in particular

$$f_k^{(k)}(r) = (-1)^{k+1} k! \log(r) + c$$

and finally $(-1)^{k+1} f_k^{(k+1)}(r) = k! r^{-1}$ which is obviously completely monotone on $(0, \infty)$. □

3 Bochner's Characterization

We saw in the last section that the Laplace transform is the right tool for analyzing positive definiteness of radial functions for all space dimensions d. However, we did not prove Schoenberg's and Micchelli's theorems. We also saw that the approach via Laplace transforms excludes functions with compact support, which are desirable from a numerical point of view. To overcome this problem and to work around these theorems, we shall now look at *translation–invariant* positive definite functions on $\mathbb{R}^d$ for some *fixed* d. We shall give the famous result of Bochner [2, 3], which characterizes translation–invariant positive definite functions via Fourier transforms. In the next section we generalize this result to handle also translation–invariant *conditionally* positive definite functions, following an approach of Madych and Nelson [11]. Of course, we define a continuous function $\Phi : \mathbb{R}^d \to \mathbb{C}$ to be a translation–invariant conditionally positive (semi–) definite function of order m on $\mathbb{R}^d$ iff $\Phi_0(x, y) := \Phi(x - y)$ is conditionally positive (semi–) definite of order m on $\mathbb{R}^d$.

Theorem 3.1 *(Bochner) A continuous function $\Phi : \mathbb{R}^d \to \mathbb{C}$ is a translation–invariant positive semi-definite function if and only if it is the inverse Fourier transform of a finite non-negative Borel measure μ on $\mathbb{R}^d$, i.e.,*

$$\Phi(x) = \mu^\vee(x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{ix^T\omega} d\mu(\omega), \qquad x \in \mathbb{R}^d. \tag{6}$$

Again, the sufficient part is easy since

$$\sum_{j,k=1}^N \alpha_j \overline{\alpha_k} \Phi(x_j - x_k) = \int_{\mathbb{R}^d} \left| \sum_{j=1}^N \alpha_j e^{ix_j^T\omega} \right|^2 d\mu(\omega), \tag{7}$$

and later we shall use this argument repeatedly to prove positive definiteness of certain functions without referring to Bochner's theorem. In the Fourier transform setting it is not straightforward to separate positive definite from positive semi-definite functions as it was in Schoenberg's characterization. But since the exponentials are linear independent on every open supset of $\mathbb{R}^d$, we have

Corollary 3.2 *Suppose that the carrier of the measure μ of Theorem 3.1 contains an open subset of $\mathbb{R}^d$. Then Φ is a translation–invariant positive definite function.*

For a complete classification of positive definite functions via Bochner's theorem see [7, 8]. Here, we want to cite a weaker formulation, which we shall not use for proving positive definiteness of special functions. A proof can be found in [18].

Theorem 3.3 *Suppose $\Phi \in L_1(\mathbb{R}^d)$ is a continuous function. Then Φ is a translation–invariant positive definite function if and only if Φ is bounded and its Fourier transform is nonnegative and not identically zero.*

Since a non–identically zero function cannot have an identically zero Fourier transform, we see that an integrable, bounded function that is not identically zero Φ is translation–invariant and positive definite if its Fourier transform is nonnegative. This can be used to prove the positive definiteness of the Gaussian along the lines of the sufficiency argument for Theorem 3.1. Since this is easily done via (7), we skip over the details and only remark that

$$\Phi(x) = e^{-\alpha\|x\|_2^2}$$

has the Fourier transform

$$\widehat{\Phi}(\omega) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \Phi(x) e^{-ix^T\omega} dx = (2\alpha)^{-d/2} e^{-\|\omega\|_2^2/(4\alpha)}. \tag{8}$$

This allows us to circumvent Schoenberg's and Bochner's theorem for a direct proof of the positive definiteness of the Gaussians (see also Powell [13]).

Now let us have a closer look at the Fourier transform of the inverse multiquadrics. To do this let us recall the definition of the modified Bessel functions. For $z \in \mathbb{C}$ with $|\arg(z)| < \pi/2$ they are given by

$$K_\nu(z) := \int_0^\infty e^{-z\cosh t} \cosh \nu t dt.$$

Theorem 3.4 *The function* $\Phi(x) = (c^2 + \|x\|_2^2)^\beta$, $x \in I\!R^d$, *with* $c > 0$ *and* $\beta < -d/2$ *is a translation–invariant positive definite function with Fourier transform*

$$\widehat{\Phi}(\omega) = \frac{2^{1+\beta}}{\Gamma(-\beta)} \left(\frac{\|\omega\|_2}{c}\right)^{-\beta-\frac{d}{2}} K_{\frac{d}{2}+\beta}(c\|\omega\|_2).$$

Proof: Since $\beta < -d/2$ the function Φ is in $L_1(I\!R^d)$. From the representation of the Gamma function for $-\beta > 0$ we see that

$$\begin{aligned} \Gamma(-\beta) &= \int_0^\infty t^{-\beta-1} e^{-t} dt \\ &= s^{-\beta} \int_0^\infty u^{-\beta-1} e^{-su} du \end{aligned}$$

by substituting $t = su$ with $s > 0$. Setting $s = c^2 + \|x\|_2^2$ this implies

$$\Phi(x) = \frac{1}{\Gamma(-\beta)} \int_0^\infty u^{-\beta-1} e^{-c^2 u} e^{-\|x\|_2^2 u} du. \tag{9}$$

Inserting this into the Fourier transform and changing the order of integration, which can be easily justified, leads to

$$\begin{aligned} \widehat{\Phi}(x) &= (2\pi)^{-d/2} \int_{I\!R^d} \Phi(\omega) e^{-ix^T\omega} d\omega \\ &= (2\pi)^{-d/2} \frac{1}{\Gamma(-\beta)} \int_{I\!R^d} \int_0^\infty u^{-\beta-1} e^{-c^2 u} e^{-\|\omega\|_2^2 u} e^{-ix^T\omega} du d\omega \\ &= (2\pi)^{-d/2} \frac{1}{\Gamma(-\beta)} \int_0^\infty u^{-\beta-1} e^{-c^2 u} \int_{I\!R^d} e^{-\|\omega\|_2^2 u} e^{-ix^T\omega} d\omega du \\ &= \frac{1}{\Gamma(-\beta)} \int_0^\infty u^{-\beta-1} e^{-c^2 u} (2u)^{-d/2} e^{-\frac{\|x\|_2^2}{4u}} du \\ &= \frac{1}{2^{d/2}\Gamma(-\beta)} \int_0^\infty u^{-\beta-\frac{d}{2}-1} e^{-c^2 u} e^{-\frac{\|x\|_2^2}{4u}} du, \end{aligned} \tag{10}$$

where we have used (8). On the other hand we can conclude from the definition of the modified Bessel function that for every $a > 0$

$$\begin{aligned} K_\nu(r) &= \frac{1}{2} \int_{-\infty}^\infty e^{-r\cosh t} e^{\nu t} dt \\ &= \frac{1}{2} \int_{-\infty}^\infty e^{-\frac{r}{2}(e^t + e^{-t})} e^{\nu t} dt \\ &= a^{-\nu} \frac{1}{2} \int_0^\infty e^{-\frac{r}{2}(\frac{s}{a} + \frac{a}{s})} s^{\nu-1} ds \end{aligned}$$

by substituting $s = ae^t$. If we now set $r = c\|x\|_2$, $a = \|x\|_2/(2c)$, and $\nu = -\beta - d/2$ we derive

$$\begin{aligned} K_{-\beta-\frac{d}{2}}(c\|x\|_2) &= \frac{1}{2}\left(\frac{\|x\|_2}{2c}\right)^{\frac{d}{2}+\beta} \int_0^\infty e^{-sc^2} e^{-\frac{\|x\|_2^2}{4s}} s^{-\beta-\frac{d}{2}-1} ds \\ &= 2^{-\beta-1}\Gamma(-\beta)\left(\frac{\|x\|_2}{c}\right)^{\frac{d}{2}+\beta} \widehat{\Phi}(x), \end{aligned}$$

which leads to the stated Fourier transform using $K_{-\nu} = K_\nu$. Since the modified Bessel function is non-negative and non-vanishing, the proof is complete. □

Note that this result is somewhat weaker than the result given in Theorem 2.3, since we require $\beta < -d/2$ for integrability reasons. Furthermore, we can read off from (9) the representing measure for Φ in the sense of Theorem 2.4.

4 The Madych–Nelson approach

So far, we have seen that the Schoenberg-Micchelli approach is an elegant way to prove conditional positive definiteness of basis functions for all space dimensions. But these characterization theorems are rather abstract, hard to prove, and restricted to globally supported and radial basis functions.

On the other hand, Bochner's characterization provides direct proofs for translation–invariant and possibly nonradial functions, but is not applicable to *conditionally* positive definite functions.

Thus in this section we follow Madych and Nelson [11] to generalize the approach of Bochner to the case of conditionally positive definite translation–invariant functions. It will turn out that the proof of the basic result is quite easy, but it will be technically difficult to apply the general result to specific basis functions. But our efforts will pay off by yielding explicit representations of generalized Fourier transforms of the classical radial basis functions, and these are important for further study of interpolation errors and stability results.

Recall that the Schwartz space $\mathcal{S}$ consists of all $C^\infty(I\!R^d)$-functions that together with all their derivatives, decay faster than any polynomial.

Definition 4.1 *For $m \in I\!N_0$ the set of all functions $\gamma \in \mathcal{S}$ which satisfy $\gamma(\omega) = \mathcal{O}(\|\omega\|_2^{2m})$ for $\|\omega\|_2 \to 0$ will be denoted by $\mathcal{S}_m$.*

Recall that a function Φ is called slowly increasing if there exists an integer $\ell \in \mathbb{N}_0$ such that $|\Phi(\omega)| = \mathcal{O}(\|\omega\|_2^\ell)$ for $\|\omega\|_2 \to \infty$.

Definition 4.2 *Suppose $\Phi : \mathbb{R}^d \to \mathbb{C}$ is continuous and slowly increasing. A continuous function $\widehat{\Phi} : \mathbb{R}^d \setminus \{0\} \to \mathbb{C}$ is said to be the generalized Fourier transform of Φ if there exists an integer $m \in \mathbb{N}_0$ such that*

$$\int_{\mathbb{R}^d} \Phi(x)\widehat{\gamma}(x)dx = \int_{\mathbb{R}^d} \widehat{\Phi}(\omega)\gamma(\omega)d\omega$$

is satisfied for all $\gamma \in \mathcal{S}_m$. The smallest of such m is called the order of $\widehat{\Phi}$.

We omit the proof that the generalized Fourier transform is uniquely defined, but rather give a first nontrivial example:

Proposition 4.3 *Suppose $\Phi = p$ is a polynomial of degree less than $2m$. Then for every test function $\gamma \in \mathcal{S}_m$ we have*

$$\int_{\mathbb{R}^d} \Phi(x)\widehat{\gamma}(x)dx = 0.$$

Proof: Suppose Φ has the representation $\Phi(x) = \sum_{|\beta|<2m} c_\beta x^\beta$. Then

$$\begin{aligned}
\int_{\mathbb{R}^d} \Phi(x)\widehat{\gamma}(x)dx &= \sum_{|\beta|<2m} c_\beta i^{-|\beta|} \int_{\mathbb{R}^d} (ix)^\beta \widehat{\gamma}(x)dx \\
&= \sum_{|\beta|<2m} c_\beta i^{-|\beta|} \int_{\mathbb{R}^d} \left(\frac{\partial^{|\beta|}\gamma}{\partial x^\beta}\right)^\wedge dx \\
&= (2\pi)^{d/2} \sum_{|\beta|<2m} c_\beta i^{-|\beta|} \frac{\partial^{|\beta|}\gamma}{\partial x^\beta}(0) \\
&= 0
\end{aligned}$$

since $\gamma \in \mathcal{S}_m$. □

Note that the above result implies that the "inverse" generalized Fourier transform is not unique, because one can add a polynomial of degree less than $2m$ to a function Φ without changing its generalized Fourier transform. Note further that there are other definitions of generalized Fourier transforms, e.g. in the context of tempered distributions.

The next theorem shows that the order of the generalized Fourier transform, which is nothing but the order of the singularity of the generalized Fourier transform at the origin, determines the minimal order of a conditionally positive definite function, provided that the function has a *nonnegative* and *nonzero* generalized Fourier transform. We will state and prove only the sufficient part, but point out that the reverse direction also holds. We need the following auxiliary result:

Lemma 4.4 *Suppose that distinct $x_1, \dots, x_N \in I\!R^d$ and $\alpha \in C^N \setminus \{0\}$ are given such that (2) is satisfied for all $p \in \pi_{m-1}(I\!R^d)$. Then*

$$\sum_{j=1}^{N} \alpha_j e^{ix_j^T \omega} = \mathcal{O}(\|\omega\|_2^m)$$

holds for $\|\omega\|_2 \to 0$.

Proof: The expansion of the exponential function leads to

$$\sum_{j=1}^{N} \alpha_j e^{ix_j^T \omega} = \sum_{k=0}^{\infty} \frac{i^k}{k!} \sum_{j=1}^{N} \alpha_j (x_j^T \omega)^k.$$

For fixed $\omega \in I\!R^d$ we have $p_k(x) := (x^T\omega)^k \in \pi_k(I\!R^d)$. Thus (2) ensures that the first $m-1$ terms vanish:

$$\sum_{j=1}^{N} \alpha_j e^{ix_j^T \omega} = \sum_{k=m}^{\infty} \frac{i^k}{k!} \sum_{j=1}^{N} \alpha_j (x_j^T \omega)^k,$$

which yields the stated behaviour. □

Theorem 4.5 *Suppose $\Phi : I\!R^d \to C$ is continuous, slowly increasing, and possesses a generalized Fourier transform $\widehat{\Phi}$ of order m which is non-negative and non-vanishing. Then Φ is a translation–invariant conditionally positive definite function of order m.*

Proof: Suppose that distinct $x_1, \dots, x_N \in I\!R^d$ and $\alpha \in C^N \setminus \{0\}$ satisfy (2) for all $p \in \pi_{m-1}(I\!R^d)$. Define

$$f(x) := \sum_{j,k=1}^{N} \alpha_j \overline{\alpha_k} \Phi(x + (x_j - x_k))$$

and

$$\gamma_\ell(x) = \left| \sum_{j=1}^{N} \alpha_j e^{ix^T x_j} \right|^2 \widehat{g}_\ell(x) = \sum_{j,k=1}^{N} \alpha_j \overline{\alpha}_k e^{ix^T(x_j - x_k)} \widehat{g}_\ell(x),$$

where $g_\ell(x) = (\ell/\pi)^{d/2} e^{-\ell\|x\|_2^2}$. On account of $\gamma_\ell \in \mathcal{S}$ and Lemma 4.4 we have $\gamma_\ell \in \mathcal{S}_m$. Furthermore,

$$\begin{aligned}
\widehat{\gamma}_\ell(x) &= (2\pi)^{-d/2} \int_{I\!R^d} \sum_{j,k=1}^{N} \alpha_j \overline{\alpha}_k e^{i\omega^T(x_j - x_k)} \widehat{g}_\ell(\omega) e^{-ix^T\omega} d\omega \\
&= \sum_{j,k=1}^{N} \alpha_j \overline{\alpha}_k (2\pi)^{-d/2} \int_{I\!R^d} \widehat{g}_\ell(\omega) e^{-i\omega^T(x-(x_j-x_k))} d\omega \\
&= \sum_{j,k=1}^{N} \alpha_j \overline{\alpha}_k g_\ell(x - (x_j - x_k)),
\end{aligned}$$

since $\widehat{\widehat{g}}_\ell = g_\ell$. Collecting these facts gives together with Definition 4.2

$$\begin{aligned}
\int_{\mathbb{R}^d} f(x) g_\ell(x) dx &= \int_{\mathbb{R}^d} \Phi(x) \sum_{j,k=1}^{N} \alpha_j \overline{\alpha_k} g_\ell(x - (x_j - x_k)) dx \\
&= \int_{\mathbb{R}^d} \Phi(x) \widehat{\gamma}_\ell(x) dx \\
&= \int_{\mathbb{R}^d} \widehat{\Phi}(\omega) \gamma_\ell(\omega) d\omega \\
&= \int_{\mathbb{R}^d} \left| \sum_{j=1}^{N} \alpha_j e^{i\omega^T x_j} \right|^2 \widehat{g}_\ell(\omega) \widehat{\Phi}(\omega) d\omega \\
&\geq 0.
\end{aligned}$$

Since Φ is only slowly increasing, we have

$$\sum_{j,k=1}^{N} \alpha_j \overline{\alpha_k} \Phi(x_j - x_k) = \lim_{\ell \to \infty} \int_{\mathbb{R}^d} f(x) g_\ell(x) dx \geq 0$$

by means of approximation by convolution. Furthermore, the quantity

$$\left| \sum_{j=1}^{N} \alpha_j e^{i\omega^T x_j} \right|^2 \widehat{g}_\ell(\omega) \widehat{\Phi}(\omega)$$

is non-decreasing in ℓ and we already know that the limit

$$\lim_{\ell \to \infty} \int_{\mathbb{R}^d} \left| \sum_{j=1}^{N} \alpha_j e^{i\omega^T x_j} \right|^2 \widehat{g}_\ell(\omega) \widehat{\Phi}(\omega) d\omega$$

exists. Hence, the limit function $(2\pi)^{-d/2} \left| \sum_{j=1}^{N} \alpha_j e^{i\omega^T x_j} \right|^2 \widehat{\Phi}(\omega)$ is integrable due to the monotone convergence theorem. Thus we have established the equality

$$\sum_{j,k=1}^{N} \alpha_j \overline{\alpha_k} \Phi(x_j - x_k) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \left| \sum_{j=1}^{N} \alpha_j e^{i\omega^T x_j} \right|^2 \widehat{\Phi}(\omega) d\omega.$$

This quadratic form cannot vanish if $\widehat{\Phi}$ is non-vanishing, since the exponentials are linearly independent. □

5 Classical Radial Basis Functions

In order to use this generalization of the Bochner approach we now compute the generalized Fourier transforms of the most popular translation–invariant or radial basis functions. Since it will turn out that these generalized Fourier transforms are non-negative and non-vanishing, we can read off the order of conditional positive definiteness of the functions from the order of the singularity of their generalized Fourier transforms at the origin.

We start with the positive definite inverse multiquadrics as treated in Theorem 3.4 and use analytic continuation to treat the case of the conditionally positive definite (non–inverse) multiquadrics. To do this we need two results on the modified Bessel functions.

Lemma 5.1 *The modified Bessel function K_ν, $\nu \in \mathbb{C}$, has the uniform bound*

$$|K_\nu(r)| \le \sqrt{\frac{2\pi}{r}} e^{-r} e^{\frac{|\Re(\nu)|^2}{2r}}, \qquad r > 0 \tag{11}$$

describing its behaviour for large r.

Proof: With $b = |\Re(\nu)|$ we have

$$\begin{aligned} |K_\nu(r)| &\le \frac{1}{2}\int_0^\infty e^{-r\cosh t}|e^{\nu t} + e^{-\nu t}|dt \\ &\le \frac{1}{2}\int_0^\infty e^{-r\cosh t}(e^{bt} + e^{-bt})dt \\ &= K_b(r) \end{aligned}$$

Furthermore, from $e^t \ge \cosh t \ge 1 + \frac{t^2}{2}$, $t \ge 0$, we can conclude

$$\begin{aligned} K_b(r) &\le \int_0^\infty e^{-r(1+\frac{t^2}{2})} e^{bt} dt \\ &\le e^{-r} e^{\frac{b^2}{2r}} \frac{1}{\sqrt{r}} \int_{\frac{-b}{\sqrt{r}}}^\infty e^{-s^2/2} ds \\ &\le \sqrt{2\pi} e^{-r} e^{\frac{b^2}{2r}} \sqrt{\frac{1}{r}}. \end{aligned}$$

□

Lemma 5.2 *For $\nu \in \mathbb{C}$ the modified Bessel function K_ν satisfies*

$$|K_\nu(r)| \le \begin{cases} 2^{|\Re(\nu)|-1}\Gamma(|\Re(\nu)|) r^{-|\Re(\nu)|}, & \Re(\nu) \ne 0, \\ \frac{1}{e} - \log\frac{r}{2}, & r < 2, \Re(\nu) = 0. \end{cases} \tag{12}$$

for $r > 0$, describing its behaviour for small r.

Proof: Let us first consider the case $\Re(\nu) \neq 0$. We set again $b = |\Re(\nu)|$ and already know that $|K_\nu(r)| \leq K_b(r)$, from the proof of the preceding lemma. Furthermore, from the proof of Theorem 3.4 we get

$$K_b(r) = \frac{1}{2} \int_0^\infty e^{-\frac{r}{2}\left(\frac{s}{a}+\frac{a}{s}\right)} \left(\frac{s}{a}\right)^b \frac{ds}{s}$$

for every $a > 0$. By setting $a = r/2$ we see that

$$K_b(r) = 2^{b-1} r^{-b} \int_0^\infty e^{-s} e^{-\frac{r^2}{4s}} s^{b-1} ds \leq 2^{b-1}\Gamma(b) r^{-b}.$$

For $\Re(\nu) = 0$ we use $\cosh t \geq e^t/2$ to derive

$$\begin{aligned} K_0(r) &= \int_0^\infty e^{-r\cosh t} dt \\ &\leq \int_0^\infty e^{-\frac{r}{2}e^t} dt \\ &= \int_{\frac{r}{2}}^\infty e^{-u} \frac{1}{u} du \\ &\leq \int_1^\infty e^{-u} du + \int_{\frac{r}{2}}^1 \frac{1}{u} du \\ &= \frac{1}{e} - \log\frac{r}{2}. \end{aligned}$$

□

We are now able to compute the generalized Fourier transform of the general multiquadrics. The basic idea of the proof goes back to Madych and Nelson [11]. It starts with the classical Fourier transform of the inverse multiquadrics as given in Theorem 3.4, and then uses analytic continuation.

Theorem 5.3 *The function $\Phi(x) = (c^2 + \|x\|_2^2)^\beta$, $x \in \mathbb{R}^d$, with $c > 0$ and $\beta \in \mathbb{R} \setminus \mathbb{N}_0$ possesses the (generalized) Fourier transform*

$$\widehat{\Phi}(\omega) = \frac{2^{1+\beta}}{\Gamma(-\beta)} \left(\frac{\|\omega\|_2}{c}\right)^{-\beta-\frac{d}{2}} K_{\frac{d}{2}+\beta}(c\|\omega\|_2), \qquad \omega \neq 0, \tag{13}$$

of order $m = \max(0, \lceil\beta\rceil)$.

Proof: Define $G = \{\lambda \in \mathbb{C} : \Re(\lambda) < m\}$ and denote the right–hand side of (13) by $\varphi_\beta(\omega)$. We are going to show by analytic continuation that

$$\int_{\mathbb{R}^d} \Phi_\lambda(\omega)\widehat{\gamma}(\omega) d\omega = \int_{\mathbb{R}^d} \varphi_\lambda(\omega)\gamma(\omega) d\omega, \qquad \gamma \in \mathcal{S}_m, \tag{14}$$

is valid for all $\lambda \in G$, where $\Phi_\lambda(\omega) = (c^2 + \|\omega\|_2^2)^\lambda$. First, note that (14) is valid for $\lambda \in G$ with $\lambda < -d/2$ by Theorem 3.4, and in case $m > 0$, also for $\lambda = 0, 1, \dots, m-1$, by Proposition 4.3 and the fact that $1/\Gamma(-\lambda)$ is zero in these cases. Analytic continuation will lead us to our stated result, if we can show that both sides of (14) exist and are analytic functions in λ. We will do this only for the right–hand side, since the left–hand side can be handled more easily. Thus we define

$$f(\lambda) = \int_{\mathbb{R}^d} \varphi_\lambda(\omega)\gamma(\omega)d\omega$$

and study this function of λ. Suppose $\mathcal{C}$ is a closed curve in G. Since φ_λ is an analytic function in $\lambda \in G$ it has the representation

$$\varphi_\lambda(\omega) = \frac{1}{2\pi i}\int_{\mathcal{C}} \frac{\varphi_z(\omega)}{z-\lambda}dz$$

for $\lambda \in \operatorname{Int}\mathcal{C}$. Now suppose that we have already shown that the integrand in the definition of $f(\lambda)$ can be bounded uniformly on $\mathcal{C}$ by an integrable function. This ensures that $f(\lambda)$ is well defined in G and by Fubini's theorem we can conclude

$$\begin{aligned} f(\lambda) &= \int_{\mathbb{R}^d} \varphi_\lambda(\omega)\gamma(\omega)d\omega \\ &= \frac{1}{2\pi i}\int_{\mathbb{R}^d}\int_{\mathcal{C}} \frac{\varphi_z(\omega)}{z-\lambda}dz\gamma(\omega)d\omega \\ &= \frac{1}{2\pi i}\int_{\mathcal{C}} \frac{1}{z-\lambda}\int_{\mathbb{R}^d} \varphi_z(\omega)\gamma(\omega)d\omega dz \\ &= \frac{1}{2\pi i}\int_{\mathcal{C}} \frac{f(z)}{z-\lambda}dz \end{aligned}$$

for $\lambda \in \operatorname{Int}\mathcal{C}$, which means that f is analytic in G. Thus it remains to bound the integrand uniformly.

Let us first consider the asymptotic behaviour in a neighbourhood of the origin, say for $\|\omega\|_2 < 1/c$. If we set $b = \Re(\lambda)$ we can use Lemma 5.2 and $\gamma \in \mathcal{S}_m$ to get in the case $b \neq -d/2$:

$$|\varphi_\lambda(\omega)\gamma(\omega)| \le C_\gamma \frac{2^{b+|b+d/2|}\Gamma(|b+d/2|)}{|\Gamma(-\lambda)|} c^{b+d/2-|b+d/2|}\|\omega\|_2^{-b-d/2-|b+d/2|+2m},$$

and in case $b = -d/2$:

$$|\varphi_\lambda(\omega)\gamma(\omega)| \le C_\gamma \frac{2^{1-d/2}}{|\Gamma(-\lambda)|}\left(\frac{1}{e} - \log\frac{c\|\omega\|_2}{2}\right)\|\omega\|_2^{2m}.$$

Since $\mathcal{C}$ is compact and $1/\Gamma$ is analytic, this gives for all $\lambda \in \mathcal{C}$

$$|\varphi_\lambda(\omega)\gamma(\omega)| \le C_{\gamma,m,c,\mathcal{C}} \left(1 + \|\omega\|_2^{-d+2\epsilon} - \log \frac{c\|\omega\|_2}{2}\right), \qquad \|\omega\|_2 \le 1/c$$

with $\epsilon = m - b > 0$. For large arguments, the integrand in the definition of $f(\lambda)$ can be estimated via Lemma 5.1 by

$$|\varphi_\lambda(\omega)\gamma(\omega)| \le C_\gamma \frac{2^{1+b}\sqrt{2\pi}}{|\Gamma(-\lambda)|} c^{b+\frac{d-1}{2}} \|\omega\|_2^{-b-\frac{d+1}{2}} e^{-c\|\omega\|_2} e^{\frac{|b+\frac{d}{2}|^2}{2c\|\omega\|_2}}$$

using that $\gamma \in \mathcal{S}$ is bounded. Since $\mathcal{C}$ is compact, this can be bounded independently of $\lambda \in \mathcal{C}$ by

$$|\varphi_\lambda(\omega)\gamma(\omega)| \le C_{\gamma,\mathcal{C},m,c} e^{-c\|\omega\|_2/2},$$

completing the proof. □

Theorem 5.4 *The function $\Phi(x) = \|x\|_2^\beta$, $x \in I\!R^d$, with $\beta > 0$, $\beta \notin 2I\!N$ has the generalized Fourier transform*

$$\widehat{\Phi}(\omega) = \frac{2^{\beta+\frac{d}{2}}\Gamma(\frac{d+\beta}{2})}{\Gamma(-\frac{\beta}{2})} \|\omega\|_2^{-\beta-d}, \qquad \omega \ne 0,$$

of order $m = \lceil \beta/2 \rceil$.

Proof: Let us start with the function $\Phi_c(x) = (c^2 + \|x\|_2^2)^{\frac{\beta}{2}}$, $c > 0$. This function possesses a generalized Fourier transform of order $m = \lceil \beta/2 \rceil$ given by

$$\widehat{\Phi}_c(\omega) = \varphi_c(\omega) = \frac{2^{1+\beta/2}}{\Gamma(-\beta/2)} \|\omega\|_2^{-\beta-d} (c\|\omega\|_2)^{\frac{\beta+d}{2}} K_{\frac{\beta+d}{2}}(c\|\omega\|_2)$$

due to Theorem 5.3. Here, we use the subscript c instead of β, since β is fixed and we want to let c go to zero. Moreover, we can conclude from the proof of Theorem 5.3 that for $\gamma \in \mathcal{S}_m$ the product can be bounded by

$$|\varphi_c(\omega)\gamma(\omega)| \le C_\gamma \frac{2^{\beta+d/2}\Gamma(\frac{\beta+d}{2})}{|\Gamma(-\beta/2)|} \|\omega\|_2^{2m-\beta-d}$$

for $\|\omega\|_2 \to 0$ and by

$$|\varphi_c(\omega)\gamma(\omega)| \le C_\gamma \frac{2^{\beta+d/2}\Gamma(\frac{\beta+d}{2})}{|\Gamma(-\beta/2)|} \|\omega\|_2^{-\beta-d}$$

for $\|\omega\|_2 \to \infty$ independently of $c > 0$. Since $|\Phi_c(\omega)\widehat{\gamma}(\omega)|$ can also be bounded independently of c by an integrable function, we can use the convergence theorem of Lebesgue twice to derive

$$\begin{aligned}
\int_{I\!R^d} \|x\|_2^\beta \widehat{\gamma}(x)dx &= \lim_{c\to 0} \int_{I\!R^d} \Phi_c(x)\widehat{\gamma}(x)dx \\
&= \lim_{c\to 0} \int_{I\!R^d} \varphi_c(\omega)\gamma(\omega)dx \\
&= \frac{2^{1+\frac{\beta}{2}}}{\Gamma(-\frac{\beta}{2})} \int_{I\!R^d} \|\omega\|_2^{-\beta-d}\gamma(\omega) \lim_{c\to 0}(c\|\omega\|_2)^{\frac{\beta+d}{2}} K_{\frac{\beta+d}{2}}(c\|\omega\|_2)d\omega \\
&= \frac{2^{\beta+d/2}\Gamma(\frac{d+\beta}{2})}{\Gamma(-\beta/2)} \int_{I\!R^d} \|\omega\|_2^{-\beta-d}\gamma(\omega)d\omega
\end{aligned}$$

for $\gamma \in \mathcal{S}_m$. The last equality follows from

$$\lim_{r\to 0} r^\nu K_\nu(r) = \lim_{r\to 0} 2^{\nu-1} \int_0^\infty e^{-t} e^{-\frac{r^2}{4t}} t^{\nu-1} dt = 2^{\nu-1}\Gamma(\nu),$$

see also the proof of Lemma 5.2. □

Theorem 5.5 *The function* $\Phi(x) = \|x\|_2^{2k} \log \|x\|_2$, $x \in I\!R^d$, $k \in I\!N$, *possesses the generalized Fourier transform*

$$\widehat{\Phi}(\omega) = (-1)^{k+1} 2^{2k-1+\frac{d}{2}} \Gamma(k + \frac{d}{2}) k! \|\omega\|_2^{-d-2k}$$

of order $m = k + 1$.

Proof: For fixed $r > 0$ and $\beta \in (2k, 2k+1)$ we expand the function $\beta \mapsto r^\beta$ using Tayloris theorem to

$$r^\beta = r^{2k} + (\beta - 2k) r^{2k} \log r + \int_{2k}^\beta (\beta - t) r^t \log r dt. \tag{15}$$

From Theorem 5.4 we know the generalized Fourier transform of the function $x \mapsto \|x\|_2^\beta$ of order $m = \lceil \beta/2 \rceil = k+1$. From Proposition 4.3 we see that the generalized Fourier transform of order m of the function $x \mapsto \|x\|_2^{2k}$ equals zero. Thus we can conclude from (15) for any test function $\gamma \in \mathcal{S}_m$ that

$$\begin{aligned}
\int_{I\!R^d} \|x\|_2^{2k} \log \|x\|_2 \widehat{\gamma}(x)dx &= \frac{1}{\beta - 2k} \int_{I\!R^d} \left(\|x\|_2^\beta - \|x\|_2^{2k} \right) \widehat{\gamma}(x)dx \\
&\quad - \frac{1}{\beta - 2k} \int_{I\!R^d} \int_{2k}^\beta (\beta - t) \|x\|_2^t \log \|x\|_2 \widehat{\gamma}(x) dt dx \\
&= \frac{2^{\beta+\frac{d}{2}}\Gamma(\frac{d+\beta}{2})}{(\beta - 2k)\Gamma(-\frac{\beta}{2})} \int_{I\!R^d} \|\omega\|_2^{-\beta-d}\gamma(\omega)d\omega \\
&\quad + \mathcal{O}(\beta - 2k)
\end{aligned}$$

for $\beta \to 2k$. Furthermore, we know from the property $\Gamma(z)\Gamma(1-z) = \pi/\sin(\pi z)$ that

$$\frac{1}{\Gamma(-\frac{\beta}{2})(\beta-2k)} = -\frac{\sin(\frac{\pi\beta}{2})\Gamma(1+\frac{\beta}{2})}{\pi(\beta-2k)}.$$

Because

$$\lim_{\beta\to 2k}\frac{\sin(\frac{\pi\beta}{2})}{\beta-2k} = \lim_{\beta\to 2k}\frac{\frac{\pi}{2}\cos(\frac{\pi\beta}{2})}{1} = \frac{\pi}{2}(-1)^k,$$

we see that

$$\lim_{\beta\to 2k}\frac{1}{\Gamma(-\frac{\beta}{2})(\beta-2k)} = (-1)^{k+1}k!/2.$$

Now we can apply the theorem of dominated convergence to derive

$$\int_{I\!R^d}\|x\|_2^{2k}\log\|x\|_2\widehat{\gamma}(x)dx = 2^{2k+d/2}\Gamma(k+d/2)(-1)^{k+1}\frac{k!}{2}\int_{I\!R^d}\|\omega\|_2^{-d-2k}\gamma(\omega)d\omega$$

for all $\gamma\in\mathcal{S}_m$, which gives the stated generalized Fourier transform. □

Now it is easy to decide whether the just investigated functions are conditionally positive definite. As mentioned before, we state the minimal m.

Corollary 5.6 *The following functions $\Phi : I\!R^d \to I\!R$ are conditionally positive definite of order m:*

- $\Phi(x) = (-1)^{\lceil\beta\rceil}(c^2+\|x\|_2^2)^\beta$, $\beta>0$, $\beta\notin 2I\!N$, $m=\lceil\beta\rceil$,
- $\Phi(x) = (c^2+\|x\|_2^2)^\beta$, $\beta<0$, $m=0$,
- $\Phi(x) = (-1)^{\lceil\beta/2\rceil}\|x\|_2^\beta$, $\beta>0$, $\beta\notin I\!N$, $m=\lceil\beta/2\rceil$,
- $\Phi(x) = (-1)^{k+1}\|x\|_2^{2k}\log\|x\|_2$, $k\in I\!N$, $m=k+1$.

6 Construction via Dimension Walk

So far we have seen that radial functions that work on $I\!R^d$ for all $d\geq 1$, are nicely characterized by the abstract results of Schoenberg and Micchelli, while translation invariant functions for fixed dimensions are best handled via Fourier transform, yielding explicit results for further use.

Here, we want to investigate radial functions for a fixed space dimension. Thus we have to take the Fourier transform, but we shall make use of radiality throughout, relying on ideas of Wu and Schaback [20], [15]. Our main goal will be the construction of compactly supported positive definite radial basis functions for fixed space dimensions.

Theorem 6.1 *Suppose $\Phi \in L_1(\mathbb{R}^d) \cap C(\mathbb{R}^d)$ is radial, i.e., $\Phi(x) = \phi(\|x\|_2)$, $x \in \mathbb{R}^d$. Then its Fourier transform $\widehat{\Phi}$ is also radial, i.e., $\widehat{\Phi}(\omega) = \mathcal{F}_d\phi(\|\omega\|_2)$ with*

$$\mathcal{F}_d\phi(r) = r^{-\frac{d-2}{2}} \int_0^\infty \phi(t) t^{\frac{d}{2}} J_{\frac{d-2}{2}}(rt)dt,$$

and ϕ satisfies $\phi(t)t^{d-1} \in L_1[0,\infty)$, in particular $\phi(t) \to 0$ for $t \to \infty$.

Proof: The case $d = 1$ follows immediately from

$$J_{-1/2}(t) = \left(\frac{2}{\pi t}\right)^{1/2} \cos t.$$

In case $d \geq 2$, splitting the Fourier integral, and using the representation

$$\int_{S_{d-1}} e^{ix^T\xi} dS(\xi) = (2\pi)^{d/2} \|x\|_2^{-\frac{d-2}{2}} J_{\frac{d-2}{2}}(\|x\|_2)$$

of the classical Bessel function J_ν via an integral over the sphere $S_{d-1} \subset \mathbb{R}^d$ yield

$$\begin{aligned}
\widehat{\Phi}(x) &= (2\pi)^{-d/2} \int_{\mathbb{R}^d} \Phi(\omega) e^{-ix^T\omega} d\omega \\
&= (2\pi)^{-d/2} \int_0^\infty t^{d-1} \int_{S_{d-1}} \phi(t\|\omega\|_2) e^{-itx^T\omega} dS(\omega) dt \\
&= (2\pi)^{-d/2} \int_0^\infty \phi(t) t^{d-1} \int_{S_{d-1}} e^{-itx^T\omega} dS(\omega) dt \\
&= r^{-(d-2)/2} \int_0^\infty \phi(t) t^{d/2} J_{(d-2)/2}(rt) dt.
\end{aligned}$$

The second assertion of the theorem follows from an inspection of the condition $\Phi \in L_1(\mathbb{R}^d)$, using the radiality of Φ. □

Theorem 6.1 gives us the opportunity to interpret the d–variate Fourier transform of a radial function via $\mathcal{F}_d$ as an operator that maps univariate functions to univariate functions.

Now let us have a closer look at this operator with respect to the space dimension. If we use $\frac{d}{dz}\{z^\nu J_\nu(z)\} = z^\nu J_{\nu-1}(z)$ we get via integration by parts, for $d \geq 3$,

$$\begin{aligned}
\mathcal{F}_d\phi(r) &= r^{-d+2} \int_0^\infty \phi(t) t \, (rt)^{\frac{d-2}{2}} J_{\frac{d-2}{2}}(rt) dt \\
&= r^{-d+2} \left(-\int_t^\infty \phi(s) s ds\right) (rt)^{\frac{d-2}{2}} J_{\frac{d-2}{2}}(rt) \Big|_{t=0}^{t=\infty} \\
&\quad + r^{-d+2} \int_0^\infty \left(\int_t^\infty \phi(s) s ds\right) r^{\frac{d}{2}} t^{\frac{d-2}{2}} J_{\frac{d-4}{2}}(rt) dt \\
&= \mathcal{F}_{d-2}\left(\int_\bullet^\infty \phi(s) s ds\right)(r)
\end{aligned}$$

whenever the boundary terms vanish. Thus if we define

$$\begin{aligned} I\phi(r) &:= \int_r^\infty \phi(t)tdt \\ D\phi(r) &:= -\frac{1}{r}\frac{d}{dr}\phi(r) \end{aligned}$$

we get the following result.

Theorem 6.2 *If $\phi \in C[0,\infty)$ satisfies $t \mapsto \phi(t)t^{d-1} \in L_1[0,\infty)$ for some $d \geq 3$, then we have $\mathcal{F}_d(\phi) = \mathcal{F}_{d-2}(I\phi)$. This means that ϕ is positive definite on $I\!R^d$ if and only if $I\phi$ is positive definite on $I\!R^{d-2}$. On the other hand, if ϕ satisfies $t \mapsto \phi(t)t^{d-1} \in L_1[0,\infty)$ for some $d \geq 1$ and if the even extension of ϕ to $I\!R$ is in $C^2(I\!R)$, then $\mathcal{F}_d(\phi) = \mathcal{F}_{d+2}(D\phi)$. In this situation, the function ϕ is positive definite on $I\!R^d$ if and only if $D\phi$ is positive definite on $I\!R^{d+2}$.*

Since both operators I and D are easily computable and satisfy $I = D^{-1}$ and $D = I^{-1}$ wherever defined, this gives us a very powerful tool for constructing positive definite functions. For example, we could start with a very smooth compactly supported function on $I\!R^1$ and apply the operator D n-times to get a positive definite and compactly supported function on $I\!R^{2n+1}$. Before we give an example, let us remark that it is possible to generalize the operators $\mathcal{F}_d$, I, D to step through the dimensions one by one and not two by two [15].

Theorem 6.3 *Define $\phi_\ell(r) := (1-r)_+^\ell$ and $\phi_{d,k}$ by*

$$\phi_{d,k} = I^k \phi_{\lfloor d/2 \rfloor + k + 1}.$$

Then $\phi_{d,k}$ is compactly supported, a polynomial within its support, and positive definite on $I\!R^d$. In particular, the function $20\phi_{3,1}(r) = (1-r)_+^4(4r+1)$ is positive definite on $I\!R^3$.

Proof: Since the operator I respects the polynomial structure and compact support, we only have to prove positive definiteness. Due to

$$\mathcal{F}_d\phi_{d,k} = \mathcal{F}_d I^k \phi_{\lfloor d/2 \rfloor + k + 1} = \mathcal{F}_{d+2k}\phi_{\lfloor (d+2k)/2 \rfloor + 1}$$

it remains to show that $\mathcal{F}_d\phi_{\lfloor d/2 \rfloor + 1}$ is nonnegative for every space dimenson d. We will follow ideas of Askey [1] to do this. Let us start with an odd dimension $d = 2n+1$. Then the Fourier transform is given by

$$r^{3n+2}\mathcal{F}_{2n+1}\phi_{n+1}(r) = \int_0^r (r-s)^{n+1} s^{n+\frac{1}{2}} J_{n-\frac{1}{2}}(s)ds.$$

Defining the right-hand side of the last equation as $g(r)$, we see that g is the convolution $g(r) = \int_0^r g_1(r-s)g_2(s)ds$ of the functions $g_1(s) := (s)_+^{n+1}$ and $g_2(s) := s^{n+1/2}J_{n-1/2}(s)$. Thus its Laplace transform $\mathcal{L}g(r) = \int_0^\infty g(t)e^{-rt}dt$ is the product of the Laplace transforms of g_1 and g_2. These transforms can be computed for $r > 0$ as

$$\mathcal{L}g_1(r) = \frac{(n+1)!}{r^{n+2}}$$

and

$$\mathcal{L}g_2(r)\frac{n!\ 2^{n+1/2}r}{\sqrt{\pi}\ (1+r^2)^{n+1}}.$$

This combines into

$$\mathcal{L}g(r) = \frac{2^{n+1/2}n!(n+1)!}{\sqrt{\pi}}\frac{1}{r^{n+1}(1+r^2)^{n+1}}.$$

On the other hand, it is well known that the function $1-\cos r$ has the Laplace transform $\frac{1}{r(1+r^2)}$. Thus, if p denotes the n-fold convolution of this function with itself, we get

$$\mathcal{L}p(r) = \frac{1}{r^{n+1}(1+r^2)^{n+1}}.$$

By the uniqueness of the Laplace transform this leads to

$$g(r) = \frac{2^{n+1/2}n!(n+1)!}{\sqrt{\pi}}p(r),$$

which is clearly nonnegative and not identically zero. For even space dimension $d = 2n$ we need only to remark that $\phi_{\lfloor\frac{2n}{2}\rfloor+1} = \phi_{\lfloor\frac{2n+1}{2}\rfloor+1}$. Hence $\phi_{\lfloor\frac{2n}{2}\rfloor+1}$ induces a positive definite function on $I\!R^{2n+1}$ and therefore also on $I\!R^{2n}$. The function $\phi(r) = (1-r)_+^4(4r+1)$ is nothing but $20\phi_{3,1}$, and hence positive definite on $I\!R^3$. □

The parameter k in the last theorem controls the smoothness of the basis function. It can be shown [17] that $\phi_{d,k}$ possesses $2k$ continuous derivatives as a radial function on $I\!R^d$ and is of minimal degree under all piecewise polynomial compactly supported functions that are positive definite on $I\!R^d$ and whose even extensions to $I\!R$ are in $C^{2k}(I\!R)$. A different technique for generating compactly supported radial basis functions is due to Buhmann [4], [5], [6].

7 Construction of general functions

So far, we have only dealt with translation–invariant (conditionally) positive definite functions, and most of our work was even restricted to radial functions. As a consequence, we had to work with basis functions that are (conditionally) positive definite on all of $I\!R^d$. In this section we want to choose a more general approach which allows us to construct positive definite functions on local domains Ω. Consequently, we have to drop Fourier and Laplace transforms, replacing them by expansions into orthogonal systems. As a byproduct, this technique allows us to construct positive definite functions on manifolds, in particular on the sphere.

Theorem 7.1 *Suppose $\Omega \subseteq I\!R^d$ is measurable. Let $\varphi_1, \varphi_2, \ldots$ be an orthonormal basis for $L_2(\Omega)$ consisting of continuous and bounded functions. Suppose that the point evaluation functionals are linearly independent on the space span $\{\varphi_j \ : \ j \in I\!N\}$. Suppose ρ_n is a sequence of positive numbers satisfying*

$$\sum_{n=1}^{\infty} \rho_n \|\varphi_n\|^2_{L_\infty(\Omega)} < \infty. \tag{16}$$

Then

$$\Phi(x, y) = \sum_{n=1}^{\infty} \rho_n \varphi_n(x) \overline{\varphi_n(y)}$$

is positive definite on Ω.

Proof: Property (16) ensures that Φ is well–defined and continuous. Furthermore, we have for $\alpha \in C\!\!\!\!I^N$ and distinct $x_1, \ldots, x_N \in \Omega$ that

$$\sum_{j,k=1}^{N} \alpha_j \overline{\alpha_k} \Phi(x_j, x_k) = \sum_{n=1}^{\infty} \rho_n \left| \sum_{j=1}^{N} \alpha_j \varphi_n(x_j) \right|^2 \geq 0.$$

Since the point evaluation functionals are linear independent on the space span $\{\varphi_j \ : \ j \in I\!N\}$, the last expression can only vanish for $\alpha = 0$. □

Note that the condition on the point evaluation functionals is somewhat unnatural for the space $L_2(\Omega)$. It would be more natural to define Φ to be positive definite, iff for every linear independent set $\Lambda = \{\lambda_1, \ldots \lambda_N\} \subseteq L_2(\Omega)^*$ and every $\alpha \in C\!\!\!\!I^N \setminus \{0\}$ the quadratic form

$$\sum_{j,k=1}^{N} \alpha_j \overline{\alpha_k} \lambda_j^x \lambda_k^y \Phi(x, y)$$

is positive. But we do not want to pursue this topic any further. Instead, we want to use Theorem 7.1 to give an example of a positive definite function on a restricted domain.

Our example deals with the space $L_2[0,2\pi]^2$ which has the bounded and continuous orthogonal basis $\{\phi_{n,k}(x_1,x_2) = e^{i(nx_1+kx_2)} \ : \ n,k \in \mathbb{Z}\}$ of functions with a 2π–periodic extension. Thus condition (16) is satisfied if the positive coefficients $\rho_{n,k}$ have the property

$$\sum_{n,k=-\infty}^{\infty} \rho_{n,k} < \infty.$$

In particular, the bivariate functions

$$\phi_{1,\ell}(x) = 1 + \sum_{(n,k)\in\mathbb{Z}^2\setminus\{0\}} \frac{1}{(n^2+k^2)^\ell} e^{i(nx_1+kx_2)}$$

and

$$\phi_{2,\ell}(x) = 1 + \sum_{\substack{n=-\infty\\ n\neq 0}}^{\infty} \frac{1}{n^{2\ell}} e^{inx_1} + \sum_{\substack{k=-\infty\\ k\neq 0}}^{\infty} \frac{1}{k^{2\ell}} e^{ikx_2} + \sum_{\substack{n=-\infty\\ n\neq 0}}^{\infty} \sum_{\substack{k=-\infty\\ k\neq 0}}^{\infty} \frac{1}{(nk)^{2\ell}} e^{i(nx_1+kx_2)}$$

generate positive definite 2π–periodic translation–invariant functions $\Phi(x,y) = \phi(x-y)$ on $[0,2\pi]^2$ for sufficiently large ℓ. Because of their tensor product structure, the latter can be computed directly (see [10]). Some examples are:

$$\begin{aligned}
\phi_{2,1}(x) &= \prod_{j=1}^{2} \left(\frac{6-\pi^2}{6} + \frac{1}{2}(x_j-\pi)^2 \right) \\
\phi_{2,2}(x) &= \prod_{j=1}^{2} \left(\frac{360-7\pi^4}{360} + \frac{\pi^2(x_j-\pi)^2}{12} - \frac{(x_j-\pi)^4}{24} \right).
\end{aligned}$$

For more examples see [10]. Of course, this tensor product approach generalizes to arbitrary space dimension, but the basic technique is much more general. See [14] for the relation to positive integral operators.

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