Characterization of Function Spaces associated to Conditionally Positive Definite Functions

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Abstract. We give a unified theory that yields three characterizations for the native function spaces associated to conditionally positive definite functions on an open subset Ω of the d dimensional Euclidean space. As a byproduct, we completely describe the dependence of the spaces on Ω.

§1. Introduction

Let $\Omega \subset \mathbb{R}^d$ be an open subset of the d-dimensional Euclidean space. We assert to interpolate function values $f(x_j) \in \mathbb{R}$ of a function $f \in C(\Omega)$ at scattered data locations $x_j \in X \subset \Omega$ by an interpolant $s_f : \Omega \to \mathbb{R}$ of the form

$$s_f(x) = \sum_{j \in J} c_j \psi(x - x_j) + p(x) \tag{1}$$

where p is in the space $\mathcal{P}_m^d$ of all polynomials with d variables of order m or less and $\psi : \mathbb{R}^d \to \mathbb{R}$ with $\psi(\cdot - x_j) \in C(\Omega)$ for all $j \in J$, is called *basis function*. Due to C. A. Micchelli's fundamental paper [7], for a finite set $X = \{x_1, \ldots, x_N\} \subset \Omega$ of pairwise distinct points with

$$p(x_j) = 0 \quad (1 \leq j \leq N) \qquad \Longrightarrow \qquad p \equiv 0 \text{ for all } p \in \mathcal{P}_m^d$$

the above interpolation problem has a unique solution under the constraints

$$\sum_{j=1}^{N} c_j p(x_j) = 0 \qquad \text{for all } p \in \mathcal{P}_m^d \tag{2}$$

provided that ψ is *conditionally positive definite of order m* on Ω:

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Definition 1.1. *A function $\psi \in C(\mathbb{R}^d)$ is conditionally positive definite of order m on Ω if the quadratic form*

$$\sum_{j,k=1}^{N} c_j c_k \psi(x_j - x_k) \tag{3}$$

is positive for all sets $X = \{x_1, \dots, x_N\} \subset \Omega$ of N pairwise distinct points and for all vectors $c = (c_1, \dots, c_N)^T \in \mathbb{R}^N \setminus \{0\}$ satisfying (2).

For *scattered data interpolation* on Ω as defined above, the conditional positive definiteness of ψ is sufficient for existence of a solution. From now on we assume ψ to be conditionally positive definite of order m on Ω. The interpolants of the form (1) subject to the condition (2) certainly form a linear space $\mathbf{F}_\psi(\Omega)$ depending on ψ and Ω. This space so far has no topology. If it is contained in some larger normed space $\mathcal{F}$ of d-variate functions, for example Sobolew space $W_\ell^n(\Omega)$, it would be interesting to calculate the $\mathcal{F}$-closure of $\mathbf{F}_\psi(\Omega)$. This would help to find error bounds for interpolants or approximants to functions f from $\mathcal{F}$ by functions in $\mathbf{F}_\psi(\Omega)$.

However, there is no such theory so far. Instead of imposing an "artificial" topology from a larger space $\mathcal{F}$ to $\mathbf{F}_\psi(\Omega)$, one can ask for more natural topologies on $\mathbf{F}_\psi(\Omega)$ that are directly related to the representation (1). Such a topology actually exists for $\Omega = \mathbb{R}^d$, dating back to early papers of Madych and Nelson [4,5,6] and conveniently described in [8]. In short, it uses (3) to define

$$|s_f|^2 := \sum_{j,k=1}^{N} c_j c_k \psi(x_j - x_k) \tag{4}$$

as a seminorm on functions of the form (1). Such a seminorm arises straightforwardly from a bilinear form, and one can take a Hilbert space closure to generate an appropriate function space $\mathcal{F}_\psi(\Omega)$. This has been done by various authors [1,2,4,5,6,8,9] in different ways, using three basic techniques:

1. variational inequalities,
2. generalized convolutions,
3. generalized Fourier transforms.

This paper serves to give a unified theory and to show that these approaches are equivalent.

Up to now, the dependence of the spaces $\mathcal{F}_\psi(\Omega)$ on Ω is not fully understood. Most authors use $\Omega = \mathbb{R}^d$ throughout, but we strictly assume a general nonempty bounded set $\Omega \subseteq \mathbb{R}^d$, having bounded domains in mind. However, our characterization results will reveal that

$$\mathcal{F}_\psi(\Omega) = \mathcal{F}_\psi(\mathbb{R}^d)\big|_{\Omega}, \tag{5}$$

proving that each function $f \in \mathcal{F}_\psi(\Omega)$ can be extended to a function in $\mathcal{F}_\psi(\mathbb{R}^d)$.

§2. Test Functions

We now add some more notation. To each function s_f of (1) there can be associated a linear functional

$$\lambda(h) := \sum_{j=1}^{N} c_j h(x_j)$$

on $C(\Omega)$ which is finitely supported and annihilates $\mathcal{P}_m^d$ due to (2). Then

$$< \lambda, \mu > := \mu^x \lambda^y \psi(x-y), \tag{6}$$

where μ^x denotes action of μ with respect to x, is a scalar product on all such functionals, and for $f_\lambda(x) := \lambda^y \psi(x-y)$ we see that $< f_\lambda, f_\mu > := < \lambda, \mu >$ is the bilinear form behind (4). Let

$$\mathcal{S} := \left\{ v \in C^\infty(\mathbb{R}^d) : \lim_{\|x\| \to \infty} \left| x^\alpha D^\beta v(x) \right| = 0 \text{ for all } \alpha, \beta \in \mathbb{N}_0^d \right\}$$

be the Schwartz space of tempered test functions. We now introduce a topology on its subset $\mathcal{S}(\Omega) := \{v \in \mathcal{S} : \text{ supp } v \subset \Omega\} \subset \mathcal{S}$ that corresponds to the one we have been considering up to now. By $\lambda_v(f) := (f, v)_{L_2(\Omega)}$ each $v \in \mathcal{S}(\Omega)$ induces a functional on the space

$$\mathcal{K}(\Omega) := \left\{ f : \Omega \to \mathbb{R} : \ \exists M \in \mathbb{N}_0 \text{ with } f(x)/(1+\|x\|)^M \in L_1(\Omega) \right\}$$

of all locally integrable functions that have at most polynomial growth on Ω. Based on (6) we define the bilinear form

$$(v, w)_\psi := \lambda_w^x \lambda_v^y \psi(x-y) \tag{7}$$

for all v, w from

$$\mathcal{S}_m^\perp(\Omega) := \left\{ v \in \mathcal{S}(\Omega) : \ \lambda_v(p) = 0 \text{ for all } p \in \mathcal{P}_m^d \right\} \subset \mathcal{S}(\Omega).$$

To be able to do this, we only require $\psi(x - \cdot), \psi(\cdot - y) \in \mathcal{K}(\Omega)$ for each $x, y \in \Omega$. But in order to prove that $\|\cdot\|_\psi := \sqrt{(\cdot,\cdot)_\psi}$ provides a norm on $\mathcal{S}_m^\perp(\Omega)$ we need some additional assumption on ψ. Following Madych and Nelson [4] and other authors using generalized Fourier transforms, we assume a continuous and *positive* function $\varphi : \mathbb{R}^d \setminus \{0\} \to \mathbb{R}$ to exist such that the representation

$$(v, w)_\psi = (2\pi)^{-d} \int_{\mathbb{R}^d} \varphi(\omega) \hat{v}(\omega) \overline{\hat{w}(\omega)} \, d\omega =: (\hat{v}, \hat{w})_\varphi \tag{8}$$

holds for all $v, w \in \mathcal{S}_m^\perp(\Omega)$. Here,

$$\hat{v}(\omega) := \int_\Omega e^{-ix^T\omega} v(x) \, dx$$

denotes the classical Fourier transform of v.

For the special case $\Omega = \mathbb{R}^d$, many standard basis functions ψ allow such a φ, but there are some examples (for instance even-order tensor-product B-splines) that induce unwanted zeros of φ. But if we assume φ to be positive, the bilinear form (7) will clearly be positive definite. This is a slightly stronger assumption than conditional positive definiteness of ψ on $\mathbb{R}^d$, because in his dissertation [3] the author proves that conditionally positive definite functions ψ on $\mathbb{R}^d$ possess a nonnegative but nonvanishing generalized Fourier transform φ in the sense of (8).

§3. Characterizations of $\mathcal{F}_\psi(\Omega)$

In this section we establish characterizations of the function space

$$\mathcal{F}_\psi(\Omega) := \left\{ f \in \mathcal{K}(\Omega) : \exists C_f \in \mathbb{R}_{\geq 0} \text{ with} |\lambda_v(f)| \leq C_f \|v\|_\psi \text{ for all } v \in \mathcal{S}_m^\perp(\Omega) \right\}.$$

Note that this definition of $\mathcal{F}_\psi(\Omega)$, which occurs in [1], [4–6] in similar form, is nothing but a characterization of functions via a variational inequality:

Theorem 3.1. *A function $f : \Omega \to \mathbb{R}$ which is locally integrable and of at most polynomial growth on Ω, is in $\mathcal{F}_\psi(\Omega)$ iff it satisfies*

$$\left| \int_\Omega f(x) v(x)\, dx \right| \leq C_f \int_\Omega \int_\Omega \psi(x-y) v(x) v(y)\, dx\, dy \quad \text{ for all } v \in \mathcal{S}_m^\perp(\Omega)$$

for some $C_f \geq 0$.

Remarks: It is allowed to replace $\mathcal{S}_m^\perp(\Omega)$ in the definition of $\mathcal{F}_\psi(\Omega)$ by $\overline{\mathcal{S}_m^\perp(\Omega)}$ because of continuity with respect to the norm $\|\cdot\|_\psi$. Doing this in Theorem 3.1 would imply a distributional interpretation of the variational inequality. Since $\mathcal{K}(\mathbb{R}^d)\big|_\Omega = \mathcal{K}(\Omega)$ and $S_m^\perp(\Omega) \subseteq S_m^\perp(\mathbb{R}^d)$ we get $\mathcal{F}_\psi(\mathbb{R}^d)\big|_\Omega \subseteq \mathcal{F}_\psi(\Omega)$ as part of (5).

For all $f \in \mathcal{F}_\psi(\Omega)$ we can define a linear functional $v \mapsto \lambda_v(f)$ on $\overline{\mathcal{S}_m^\perp(\Omega)}$. By the theorem of Fischer-Riesz there is a unique $v_f \in \overline{\mathcal{S}_m^\perp(\Omega)}$ such that $\lambda_v(f) = (v_f, v)_\psi$ for all $v \in \overline{\mathcal{S}_m^\perp(\Omega)}$. Now $\Lambda : \mathcal{F}_\psi(\Omega) \to \overline{\mathcal{S}_m^\perp(\Omega)}$ with $\Lambda(f) = v_f$ is a linear mapping with

$$\mathcal{P}_m^d(\Omega) := \left\{ f : \Omega \to \mathbb{R} : \; \exists p \in \mathcal{P}_m^d \text{ with } f \equiv p|_\Omega \right\} \subset \ker \Lambda.$$

The other inclusion follows from [5], Lemma 3.2. We now show surjectivity of Λ. Choosing an arbitrary $w \in \mathcal{S}_m^\perp(\Omega)$ we consider the function $f_w := \psi * w$. Using

$$|\lambda_v(f_w)| = |\lambda_v(\psi * w)| = |\lambda_v^x \lambda_w^y \psi(x-y)| = \left| (w, v)_\psi \right| \leq \|w\|_\psi \cdot \|v\|_\psi \tag{9}$$

for all $v, w \in \mathcal{S}_m^\perp(\Omega)$ we realize that f_w coincides on Ω with a function $f_{w,\Omega}$ which is in $\mathcal{F}_\psi(\Omega)$ by definition. We have a linear map $V : \mathcal{S}_m^\perp(\Omega) \to \mathcal{F}_\psi(\Omega)$

with $V(w) = f_{w,\Omega}$ and $\lambda_v(V(w)) = \lambda_v^x \lambda_w^y \psi(x-y) = (w,v)_\psi$ for all $v, w \in \mathcal{S}_m^\perp(\Omega)$, and this generalizes to $\overline{\mathcal{S}_m^\perp(\Omega)}$ by (9) and continuity. Note that both V and Λ are isometric, if a suitable norm is defined in $\mathcal{F}_\psi(\Omega)$.

Checking $\Lambda \circ V$ we find that

$$((\Lambda \circ V)(w), v)_\psi = \lambda_v(V(w)) = (w,v)_\psi$$

for all $v, w \in \overline{\mathcal{S}_m^\perp(\Omega)}$, implying that $\Lambda \circ V$ is the identity on $\overline{\mathcal{S}_m^\perp(\Omega)}$ and Λ is surjective. This yields $\overline{\mathcal{S}_m^\perp(\Omega)} \cong \mathcal{F}_\psi(\Omega)/\mathrm{ker}\Lambda = \mathcal{F}_\psi(\Omega)/\mathcal{P}_m^d(\Omega)$ and a characterization of $\mathcal{F}_\psi(\Omega)$ via generalized convolution:

Theorem 3.2. *(cf. [2])*

$$\mathcal{F}_\psi(\Omega) = \mathcal{P}_m^d(\Omega) \bigoplus V(\overline{\mathcal{S}_m^\perp(\Omega)}). \tag{10}$$

In particular, $\mathcal{F}_\psi(\Omega)$ consists of $\mathcal{P}_m^d(\Omega)$ plus all functions $f_{w,\Omega}$ generated by limits of convolutions

$$(\psi * w_n)(x) = \int_\Omega \psi(x-y) w_n(y)\, dy$$

for $w_n \in \mathcal{S}_m^\perp(\Omega)$ under convergence in $\|\cdot\|_\psi$.

Note that (10) immediately implies $\mathcal{F}_\psi(\Omega) \subseteq \mathcal{F}_\psi(\mathbb{R}^d)\big|_\Omega$, proving (5). Except for our motivation of the introduction of φ, we did not use Fourier transforms so far. But from (10) we can write any $f_\Omega \in \mathcal{F}_\psi(\Omega)$ as $f_\Omega = p_\Omega + f_{w,\Omega}$ with $p_\Omega \in \mathcal{P}_m^d(\Omega)$ and $f_{w,\Omega} = V(w)$ for $w \in \overline{\mathcal{S}_m^\perp(\Omega)}$, and extend it canonically to a function $f = p + \psi * w : \mathbb{R}^d \to \mathbb{R}$. Now we can take distributional Fourier transforms of both p and $f_w = \psi * w$. The latter is treated by

$$F(f_w) = F(\psi * w) = F(\psi) \cdot \hat{w} = \varphi \cdot \hat{w}$$

for $w \in \mathcal{S}_m^\perp(\Omega)$, where F denotes the distributional Fourier transform. For $w \in \overline{\mathcal{S}_m^\perp(\Omega)}$ we can only resort to the distributional interpretation

$$\lambda_{\hat{v}}(F(f_w)) := \lambda_v(f_w) = \lambda_v^x \lambda_w^y \psi(x-y) = (w,v)_\psi = (\hat{w}, \hat{v})_\varphi$$

for all $v \in \overline{\mathcal{S}_m^\perp(\Omega)}$. Here, we tacitly extended the Fourier transform to $\overline{\mathcal{S}_m^\perp(\Omega)}$ by continuity. If we interpret this in $L_2(\mathbb{R}^d)$, we find that by

$$(\varphi \cdot \hat{w})(\hat{v}) := (\hat{w}, \hat{v})_\varphi \qquad \text{for all } v \in \overline{\mathcal{S}_m^\perp(\Omega)}$$

the identity $F(f_w) = \varphi \cdot \hat{w}$ holds as an identity of functionals. If understood in a generalized sense, we have the third characterization of functions in $\mathcal{F}_\psi(\Omega)$:

Theorem 3.3. *(cf. [1,4,6]) The space $\mathcal{F}_\psi(\Omega)$ consists of polynomials from $\mathcal{P}_m^d(\Omega)$ plus functions from $\mathcal{K}(\Omega)$ which are restrictions to Ω of functions defined on $\mathbb{R}^d$ whose generalized Fourier transforms are a product of φ with a function in the weighted L_2 space*

$$\mathcal{L}_\varphi^2 := \left\{ f : \mathbb{R}^d \to \mathbb{R} : \int_{\mathbb{R}^d} |f(\omega)|^2 \varphi(\omega)\, d\omega < \infty \right\}.$$

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