Characterization of semi-Hilbert Spaces with Application in Scattered Data Interpolation

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Abstract. Conditionally positive definite functions, in particular radial basic functions, and associated native Hilbert spaces have been extensively studied for the case where the native Hilbert space consists of continuous functions. In this paper we extend both concepts to what we call semi-Hilbert kernel and semi-Hilbert space in the context of locally convex vector spaces for which the well-known case is a special example. We discuss the relation between semi-Hilbert kernels and semi-Hilbert spaces. We further study generalized minimal semi-norm interpolation and state necessary and sufficient conditions for unique solutions. This covers many interpolation problems encountered in practice, in particular, optimal recovery from generalized Hermite-Birkhoff data given as an example.

§1. Introduction

In this article we pick up on the abstract kernel theory for quotient spaces, briefly introduced in J. Duchon’s seminal paper [4], extend the framework, and derive new results on semi-Hilbert spaces and minimal semi-norm interpolation. Remarkably, the quotient space approach, fundamental to Duchon’s surface spline theory, has not received much attention except by P.-J. Laurent in the context of quadratic convex analysis [7]. However, there have been several attempts to continue the work on surface splines. The most well-known is Madych and Nelson’s study on conditionally positive definite functions and associated native spaces, a concept which has been further investigated by R. Schaback in [13]. Madych and Nelson considered a less transparent Hilbert space approach [9] on one hand, and a more technical Fourier analysis approach [10] on the other hand in order to derive their results without making use of the general Hilbert kernel
theory developed by L. Schwartz [15]. This general Hilbert kernel theory, however, provides a natural framework to study and extend what has been initiated in [4]. It includes Madych and Nelson’s work as a special example.

We will make use of L. Schwartz’ seminal article throughout this paper. The approach is heavily based on classical topological vector space theory. We will not explicitly present definitions and standard arguments of this discipline, but rather refer to excellent books such as [14] and [16].

Before we give a brief overview of Schwartz’ Hilbert kernel theory, it is worth mentioning that Duchon’s idea of applying Hilbert kernel theory to quotient spaces represents another case of general spline theory which has been the subject of many research articles in the late sixties, e.g., [1] and [6], and early seventies, e.g., [2] and [8], but which has lost its battle against numerical analysis and computational science, vitalized by the availability of increasingly powerful computer systems.

§2. Characterization of Semi-Hilbert Spaces

In what follows, $E$ always denotes a locally convex quasi-complete Hausdorff space over $\mathbb{R}$ as, for example, the linear space of $k$-times continuously differentiable functions $C^k$ endowed with the topology of uniform convergence on compact subsets of the functions and their derivatives of order $\leq k$, see [16].

Let $E'$ be the topological dual of $E$ containing all continuous functionals on $E$. For $e' \in E'$ acting on $e \in E$, we write $\langle e', e \rangle$.

We first outline the central results of Schwartz’ Hilbert kernel theory.

**Definition 1.** A kernel $\kappa$ relative to $E$ is a linear map of $E'$ to $E$ which is continuous for the weak topologies $\sigma(E', E)$ and $\sigma(E, E')$.

A kernel $\kappa$ relative to $E$ is positive if

$$\langle e', \kappa e' \rangle \geq 0, \quad (e' \in E').$$

The set of all positive kernels is denoted by $\mathbb{L}(E)$.

**Definition 2.** A subspace $H$ of $E$ endowed with an inner product $(\cdot | \cdot)_H$ is called a Hilbert subspace of $E$ if $H$ is complete, and if the natural inclusion $j : H \to E$ is continuous.

For the set of all Hilbert subspace of $E$ we write $\mathbb{H}(E)$. We further denote by $\nu$ the canonical Riesz map of a Hilbert space $H$ mapping $H'$ into $H$. The transpose of an operator is indicated with the upper script symbol $^t$.

The following results stated in [15] can be easily deduced from classical functional analysis.
**Proposition 3.** Let $H$ be a Hilbert subspace of $E$. Then, $\kappa = j\nu j^t$ is the unique map of $E'$ to $H$ such that

$$(h|\kappa e') = \langle e', h \rangle,$$

$$(e' \in E', h \in H).$$

The range of $\kappa$ is dense in $H$ and $\kappa$ is a positive kernel relative to $E$.

**Definition 4.** For $H \in \mathbb{H}(E)$, we call $\kappa = j\nu j^t$ the Hilbert kernel of $H$.

**Proposition 5.** Let $\kappa$ be the Hilbert kernel of $H \in \mathbb{H}(E)$. The following statements are equivalent.

1) $H$ is dense in $E$.

2) $\kappa$ is one-to-one.

3) $\langle e', \kappa e' \rangle > 0$ for all $e' \neq 0$.

The main result of [15] is the following.

**Theorem 6.** The mapping $\mathbb{H}(E) \to \mathbb{L}(E)$ is bijective.

Because of its generality, L. Schwartz’ kernel theory can be applied to quotient spaces. This is the main idea when dealing with bi-linear forms that are not positive definite.

Throughout the paper, let $N$ be a finite dimensional subspace of $E$ and $\pi$ a continuous projection onto $N$. Then, $E$ can be split into a direct sum of the closed subspaces $V = \ker(\pi)$ and $N$, see, for example, [16]. From the direct sum we can easily deduce that the quotient space $E/N$ inherits all topological properties from $E$. In particular, $E/N$ is also a locally convex quasi-complete Hausdorff space and we can give the following definition.

**Definition 7.** A subspace $S$ of $E$ is called a semi-Hilbert subspace of $E$ with nullspace $N$ if $S$ is endowed with a non-negative bi-linear form $(\cdot|\cdot)_S$ which defines a semi-norm on $S$ with finite dimensional nullspace $N$ such that $S/N$ endowed with the quotient norm is a Hilbert subspace of $E/N$.

The set of all semi-Hilbert subspaces of $E$ with nullspace $N$ is denoted by $\mathbb{H}(E,N)$. Definition 7 coincides with what is called semi-Hilbertian space in [7]. It first appeared in [4]. If $\rho$ denotes the canonical quotient map, then the definition implies $(x|y)_S = (\rho x|\rho y)_{S/N}$.

The orthogonal complement of $N$ with respect to $E$ is defined by

$N^\perp = \{ e' \in E' : \langle e', e \rangle = 0, \ e \in N \}.$

In case of ambiguity, we also write $N^\perp e'$.

**Definition 8.** A semi-Hilbert kernel $\sigma$ of $E$ relative to $N$ is a weakly continuous linear map of $E'$ to $E$ such that

$$\langle e', \sigma e' \rangle \geq 0, \quad (e' \in N^\perp).$$

Similar to Theorem 6, we can characterize semi-Hilbert subspaces in terms of semi-Hilbert kernels.
Theorem 9. For a semi-Hilbert kernel $\sigma$ of $E$ relative to $N$, there exists a unique semi-Hilbert subspace $S \in \mathbb{H}(E, N)$ such that $\sigma(N^\perp) \subset S$ and
\[
(x \mid \sigma e')_S = \langle e', x \rangle, \quad (x \in S, \ e' \in N^\perp).
\] (1)
In this case, $\sigma$ is said to be a semi-Hilbert kernel of $S$.

Proof: It can easily be seen that the linear map $\rho_\sigma \rho'$ is a Hilbert kernel relative to $E/N$ which induces a unique Hilbert subspace $H$. The reciprocal image of $H$ with respect to $\rho$ is a semi-Hilbert subspace of $E$ with semi-Hilbert kernel $\sigma$. The uniqueness of $S$ follows from the uniqueness of $H$.

Theorem 10. Let $S$ be a semi-Hilbert subspace of $E$ with nullspace $N$. Then, there exists a semi-Hilbert kernel $\sigma$ of $S$. If $\tilde{\sigma}$ is another semi-Hilbert kernel of $S$, then $(\sigma - \tilde{\sigma})(N^\perp) \subset N$. In particular, $\langle e', \sigma e' \rangle = \langle e', \tilde{\sigma} e' \rangle$ for all $e' \in N^\perp$.

Proof: Similar to $E = V \oplus N$, where $V = \ker(\pi)$, we have $S = K \oplus N$ with $K = S \cap V$. The bi-linear form $(\cdot \mid \cdot)_S$ restricted to $K$ turns into an inner product and makes $K$ a Hilbert subspace of $E$. Its unique Hilbert kernel is one possible semi-Hilbert kernel of $S$, say $\sigma$. From the properties of a semi-Hilbert kernel of $S$ it follows that if $\tilde{\sigma}$ is another semi-Hilbert kernel of $S$, then $(\sigma - \tilde{\sigma})(N^\perp) \subset N$. □

The following results are simple consequences of the argument applied in the above proof.

Proposition 11. Let $S \in \mathbb{H}(E, N)$ with semi-Hilbert kernel $\sigma$, and let $\pi$ be a continuous projection of $E$ onto $N$ with complementary projection $q$. The unique Hilbert kernel of $K = S \cap \ker(\pi) \in \mathbb{H}(E)$ is given by $q \sigma q'$.

Proposition 12. Let $S$ be in $\mathbb{H}(E, N)$, and let $\pi$ be a continuous projection of $E$ onto $N$ inducing the Hilbert subspace $K = S \cap \ker(\pi)$ of $E$ endowed with $(\cdot \mid \cdot)_S$. Assume that $F$ is a locally convex separated space and $N$ is a subspace of $F$. If $K \in \mathbb{H}(F)$, then $S \in \mathbb{H}(F, N)$.

§3. Interpolation of a Finite Data Set

Let $M$ be a finite dimensional, hence closed, subspace of $E'$. The orthogonal complement of $M$ is defined by $\perp M = \{e \in E : \langle e', e \rangle, \ e' \in M\}$. Recall that $\rho'$ is a topological isomorphism from $(E/N)'$ to $N^\perp$, see [16].

Lemma 13. Let $S \in \mathbb{H}(E, N)$. Then,
\[
\rho(\perp M \cap S) = \perp(\rho^{-1}(M \cap N^\perp)) \cap S/N.
\]

Proof: The set equality follows from simple properties of orthogonal sets and the observation that $\perp (M \cap N^\perp) = \perp M + \perp N = \perp M + N$. □

We state the non-constructive part of the minimal semi-norm interpolation in a semi-Hilbert subspace.
Theorem 14. Let $S$ be in $\mathbb{H}(E, N)$, and let $M$ be a finite dimensional subspace of $E'$. For $x_0 \in S$, there exists a minimal semi-norm element $x_M \in S$ interpolating $x_0$ for $M$, i.e., $\langle e', x_M \rangle = \langle e', x_0 \rangle$ for all $e' \in M$. Two such elements differ only by an element of $N$.

Proof: Every element in $S$ interpolating $x_0$ for $M$ is in the affine subspace $x_0 + \perp M \cap S$. Lemma 13 implies that $\rho x_0 + \rho(\perp M \cap S)$ is closed in $S/N$ and, therefore, contains a unique minimal norm element which in turn contains at least one element in $x_0 + \perp M \cap S$, say $x_M$. The element $x_M$ interpolates $x_0$ for $M$ and has minimal semi-norm. Any other such element must be in the same equivalence class. □

From Theorem 14 it can easily be seen that if we assume

$$\perp M \cap N = \{0\},$$

then the minimal semi-norm interpolation is unique. We call $M$ satisfying (2) unisolvent for $N$. The following is referred to as the constructive part of the minimal semi-norm interpolation.

Theorem 15. For $S \in \mathbb{H}(E, N)$ with semi-Hilbert kernel $\sigma$, $M$ a finite dimensional subspace of $E'$, any minimal semi-norm interpolation $x_M$ of some $x_0 \in S$ for $M$ is element of $\sigma(M \cap N^\perp) + N$.

Proof: Let $\kappa$ be the Hilbert kernel of $S/N$ which is given by $\kappa = \rho \sigma \rho^t$. As $\rho x_M$ is the minimal norm element of the affine subspace $\rho x_0 + \rho(\perp M \cap S)$ it follows that $\rho x_M$ is in $\rho(\perp M \cap S)^\perp$, where $\perp$ denotes the orthogonal complement in the Hilbert space $S/N$. Applying Lemma 13 and the fact that $\kappa = j\nu j^t$, we deduce that

$$\rho(\perp M \cap S)^\perp = (\perp(\rho^{-t}(M \cap N^\perp)) \cap S/N)^\perp$$

$$\quad = \nu((\perp(\rho^{-t}(M \cap N^\perp)) \cap S/N)^\perp')$$

$$\quad = \nu j^t(\rho^{-t}(M \cap N^\perp)) = \kappa \rho^{-t}(M \cap N^\perp) = \rho \sigma (M \cap N^\perp).$$

The proof is complete. □

Both the non-constructive and the constructive part are well-known results, see, for example, [7]. The proofs given here, however, emphasize the role of the semi-Hilbert kernel.

Because of (1), it is clear that for $x_M$ in $\sigma(M \cap N^\perp) + N$, there exists a unique pair $(e', e) \in M \cap N^\perp \times N$ such that $x_M = \sigma e' + e$ if and only if $M$ is unisolvent for $N$ and $\langle e', \sigma e' \rangle > 0$ for all nonzero elements $e' \in M \cap N^\perp$. We call a semi-Hilbert kernel $\sigma$ strictly positive if $\langle e', \sigma e' \rangle > 0$ for all nonzero $e' \in N^\perp$. 
Theorem 16. Let $S$ be an element of $\mathbb{H}(E, N)$ with semi-Hilbert kernel $\sigma$. Then, $\sigma$ is strictly positive if and only if $S$ is dense in $E$.

Proof: Let $\kappa$ be the Hilbert kernel of $S/N$. It can easily be seen that $\sigma$ is strictly positive if and only if $\kappa$ is strictly positive, i.e., $\langle e', \kappa e' \rangle > 0$ for all nonzero $e' \in (E/N)'$. Proposition 5 says that $\kappa$ be strictly positive is equivalent to $S/N$ be dense in $E/N$. But the latter holds if and only if $S$ is dense in $E$. The proof is complete. □

§4. Semi-reproducing Kernels

We discuss the case of semi-Hilbert spaces of $E = \mathbb{R}^\Omega$, $\Omega \subset \mathbb{R}^d$ with nullspace $N = P^d_r$, the set of $d$-variate polynomials of maximal order $r$ which is of finite dimension, say $Q$. When endowing $E$ with the topology of pointwise convergence, $E$ turns into a locally convex complete Hausdorff space. The dual is spanned by the set of point measures $\delta_x$, $x \in \Omega$.

Let $\sigma$ be a semi-Hilbert kernel of $E$ relative to $N$. It uniquely determines the function

$$\Phi(x, \xi) = \langle \delta_x, \sigma \delta_\xi \rangle, \quad (x, \xi \in \Omega).$$

This is what is usually called a conditionally positive definite function of order $r$. It generates a semi-Hilbert space $S$ of $E$ with nullspace $N$, also known as the native space of $\Phi$, see [13]. We call $\Phi$ a semi-reproducing kernel of $S$.

Assume that there exists a point set $\xi_1, \ldots, \xi_Q$ in $\Omega$ such that the set $\{\delta_{\xi_1}, \ldots, \delta_{\xi_Q}\}$ is unisolvent for $N$. Then we can define a continuous projection $\pi$ of $E$ onto $N$ by

$$\pi = \sum_{j=1}^Q p_j \delta_{\xi_j}, \quad (3)$$

where $p_1, \ldots, p_Q$ are the Lagrange polynomials with respect to $\xi_1, \ldots, \xi_Q$. By Proposition 12 we have that $K = S \cap \ker(\pi)$ is a Hilbert subspace of $E$ with Hilbert kernel $\kappa = q^t \delta_x$, where $q$ is the complementary projection of $\pi$. We define

$$\delta(x) = q^t \delta_x$$

as introduced in [11]. It easily follows that $\delta(x)$ is in $N^\perp$. It is also easy to show that the reproducing kernel $A(x, \xi) = \langle \delta_x, \kappa \delta_\xi \rangle$ of $K$ as defined in [15] satisfies

$$A(x, \xi) = \langle \delta(x), \sigma \delta(\xi) \rangle$$

which implies the kernel relation $A(x, \xi) = \Phi(x, \xi) - \sum_{j=1}^Q (\Phi(x, \xi_j)p_j(\xi) + \Phi(\xi_j, \xi)p_j(x) - \sum_{k=1}^Q \Phi(\xi_j, \xi_k)p_j(x)p_k(\xi))$, as also derived in [13]. Using Schwartz’s theorems on reproducing kernels we arrive at the following results.
Theorem 17. Let $\Phi$ be the semi-reproducing kernel induced by the semi-Hilbert kernel $\sigma$ of $S \in \mathbb{H}(E, N)$. If $\Phi$ is separately continuous and locally bounded on $\Omega \times \Omega$, then $S$ is a semi-Hilbert subspace of $C(\Omega)$ with nullspace $N$. By setting
\[ \sigma \mu = \mu^\xi \Phi(\cdot, \xi), \quad (\mu \in C') \]
the semi-Hilbert kernel $\sigma$ extends to a semi-Hilbert kernel of $C(\Omega)$ relative to $N$ with semi-Hilbert subspace $S$.

Proof: Let $\pi$ be defined as in (3) with complementary projection $q$ and $K = S \cap \ker(\pi)$ the corresponding Hilbert subspace of $E$. By the kernel relation, the reproducing kernel $A$ of $K$ is separately continuous and locally bounded. From [15] it follows that $K$ is a Hilbert subspace of $C(\Omega)$, and the first claim follows from Proposition 12. For the second claim, observe that
\[ \langle \mu, \sigma \mu \rangle = \mu^\xi \mu^\xi \Phi = \mu^\xi \mu^\xi A = \langle \mu, \kappa \mu \rangle \geq 0, \quad (\mu \in N^\perp_{C'}) \]
which implies that $\sigma$ is a semi-Hilbert kernel of $C(\Omega)$ relative to $N$. It remains to show that $\sigma$ induces $S$. But this follows from the fact that
\[ \sigma \mu = (q + \pi)\mu^\xi \Phi = q(\mu^\xi \Phi) + \pi(\mu^\xi \Phi) = q(\mu^\xi A) + \pi(\mu^\xi \Phi) \]
is in $K + N \subset S$ for all $\mu \in N^\perp_{C'}$, and from the fact that
\[ \langle \mu, g \rangle = \langle \mu, q g \rangle = (q g|\kappa \mu)_K = (g|\sigma \mu)_S, \]
for all $g \in S$ and $\mu \in N^\perp_{C'}$. The proof is complete. \qed

The same arguments yield the following theorem.

Theorem 18. Let $k$ be an integer $\geq 1$ and $\Omega$ open. Let $\Phi$ be the semi-reproducing kernel induced by the semi-Hilbert kernel $\sigma$ of $S \in \mathbb{H}(E, N)$. If $\sum_{|\alpha|=k} D_\alpha^\alpha D_\xi^\xi \Phi$, in the distributional sense, is a separately continuous and locally bounded function on $\Omega \times \Omega$, then $S$ is a semi-Hilbert subspace of $C^k(\Omega)$ with nullspace $N$. By setting
\[ \sigma T = T^\xi \Phi(\cdot, \xi), \quad (T \in (C^k)^'), \]
the semi-Hilbert kernel $\sigma$ extends to a semi-Hilbert kernel of $C^k(\Omega)$ relative to $N$ with semi-Hilbert subspace $S$.

Similar results hold if we take for $E$ the set of distributions $D'$ on an open subset of $\mathbb{R}^d$. If the semi-reproducing kernel $\Phi$ depends only on the difference $x - \xi$ then $S$, but not $K$, is translation invariant. In this case, Fourier analysis can be applied as used in [10] and [5].
Assume that for some $k \geq 1$, $\Phi$ satisfies the conditions of Theorem 18. Assume further that $S$ contains a subset which is dense in $C^k$. Let $M$ be spanned by linearly independent $T_1, \ldots, T_n \in (C^k)'$, and let $M$ be unisolvent for $N$. Then, for any data vector $\gamma \in \mathbb{R}^n$, there exists a unique minimal semi-norm element $s_M$ in $S$ interpolating $\gamma$ for $T_1, \ldots, T_n$. By Theorem 15, $s_M$ is of the form

$$s_M(\cdot) = \sum_{j=1}^{n} b_j T_j^\xi \Phi(\cdot, \xi) + \sum_{k=1}^{Q} c_k p_k(\cdot),$$

where the coefficients satisfy the linear system

$$Bb + Pc = \gamma, \quad P^t c = 0$$

with the matrices $B = (T_x^i T_j^\xi \Phi)$ and $P = (T_i p_k)$. The statement follows from the fact that the square system matrix is invertible since both assumptions (i) $S$ is dense in $C^k$ and (ii) $T_1, \ldots, T_n$ are linearly independent, assure that the homogeneous system allows only the trivial solution.

§5. Examples

One of the most well-known examples of conditionally positive definite functions are Duchon’s surface splines

$$\Phi_k(x, \xi) = \|x - \xi\|^{2k-1}, \quad \text{if } d \text{ is odd},$$

$$\Phi_k(x, \xi) = \|x - \xi\|^{2k} \log(\|x - \xi\|), \quad \text{if } d \text{ is even},$$

where $\|\cdot\|$ is the Euclidean norm in $\mathbb{R}^d$ and $k = 1, 2, \ldots$ is the order of the surface spline. In order to verify that $\Phi_k$ is conditionally positive definite of order $r = k + \lfloor d/2 \rfloor$ we can use Micchelli’s theorem for radial functions [12]. It is not difficult to see that

$$\sum_{|\alpha| = k-1} D_x^\alpha D_\xi^\alpha \Phi_k$$

is continuous, and hence the induced semi-Hilbert space is a subspace of $C^{k-1}(\mathbb{R}^d)$. As it can be seen, for example, from Duchon’s work, these semi-Hilbert spaces coincide with the Beppo-Levi spaces endowed with the rotational invariant semi-norm

$$\|f\|_r = \left( \sum_{|\alpha| = r} \frac{r!}{\alpha!} \int_{\mathbb{R}^d} |D^\alpha f(x)|^2 dx \right)^{1/2}$$

for which the Sobolev Lemma yields the same smoothness properties as just derived, see, for example, [3].
If we want to interpolate Hermite-Birkhoff data in $\mathbb{R}^2$ consisting of point-values and derivatives up to order $k - 1$, we have to take, at least, $\Phi_k$ or higher order surface splines. Figure 1 shows a simple example of minimal semi-norm interpolation in the plane. For the local extreme values we interpolate the second derivatives of the Hesse matrix such that it becomes positive definite, negative definite, or indefinite, respectively.

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