

Native Hilbert Spaces for Radial Basis Functions I

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Abstract

This contribution gives a partial survey over the native spaces associated to (not necessarily radial) basis functions. Starting from reproducing kernel Hilbert spaces and invariance properties, the general construction of native spaces is carried out for both the unconditionally and the conditionally positive definite case. The definitions of the latter are based on finitely supported functionals only. Fourier or other transforms are not required. The dependence of native spaces on the domain is studied, and criteria for functions and functionals to be in the native space are given. Basic facts on optimal recovery, power functions, and error bounds are included.

1 Introduction

For the numerical treatment of functions of many variables, *radial basis functions* are useful tools. They have the form $\phi(\|x - y\|_2)$ for vectors $x, y \in \mathbb{R}^d$ with a *univariate* function ϕ defined on $[0, \infty)$ and the Euclidean norm $\|\cdot\|_2$ on \mathbb{R}^d . This allows to work efficiently for large dimensions d , because the function boils the multivariate setting down to a univariate setting. Usually, the multivariate context comes back into play by picking a large number M of points x_1, \dots, x_M in \mathbb{R}^d and working with linear combinations

$$s(x) := \sum_{j=1}^M \lambda_j \phi(\|x_j - x\|_2).$$

In certain cases, low-degree polynomials have to be added, but we give details later. Typical examples for radial functions $\phi(r)$ on $r = \|x - y\|_2$, $x, y \in \mathbb{R}^d$ are

$$\begin{aligned}
\text{thin-plate splines: } & r^\beta \log r, \beta > 0, \beta \in 2\mathbb{N} \quad [1] \\
& r^\beta, \beta > 0, \beta \notin 2\mathbb{N} \quad [1] \\
\text{multiquadrics: } & (r^2 + c^2)^{\beta/2}, \beta > 0, \beta \notin 2\mathbb{N} \quad [6] \\
\text{inverse multiquadrics: } & (r^2 + c^2)^{\beta/2}, \beta < 0, \quad [6] \\
\text{Gaussians: } & \exp(-\beta r^2), \beta > 0, \\
\text{Sobolev splines: } & r^{k-d/2} K_{k-d/2}(r), \quad k > d/2 \\
\text{Wendland function: } & (1 - r)_+^4 (1 + 4r), d \leq 3
\end{aligned}$$

Another important case are *zonal* functions on the $(d - 1)$ -dimensional sphere $S^{d-1} \subset \mathbb{R}^d$. These have the form $\phi(x^T y) = \phi(\cos(\alpha(x, y)))$ for points x, y on the sphere spanning an angle of $\alpha(x, y) \in [0, \pi]$ at the origin. Here, the symbol T denotes vector transposition, and the function ϕ should be defined on $[-1, 1]$. Periodic multivariate functions can also be treated, e.g. by reducing them to products of univariate periodic functions.

All of these cases of *basis functions* share a common theoretical foundation which forms the main topic of this paper. The functions all have a unique associated “native” Hilbert space of functions in which they act as a generalized reproducing kernel. The different special cases (radiality, zonality) are naturally related to geometric invariants of the native spaces. The paper will thus start in section 2 with reproducing kernel Hilbert spaces and look at geometric invariants later in section 3.

But most basis functions are constructed directly and do not easily provide information on their underlying native space. Their main properties are symmetry and (strict) positive definiteness (SPD) or conditionally positive definiteness (CPD). These notions are defined without any relation to a Hilbert space, and we then have to show how to construct the native space, prove its uniqueness, and find its basic features. We do this for SPD functions in section 4 and for CPD functions in section 5. The results mostly date back to classical work on reproducing kernel Hilbert spaces and positive definite functions (see e.g. [12], [17]). We compile the necessary material here to provide easy access for researchers and students. Some new results are included, and open problems are pointed out. In particular, we show how to modify the given basis function in order to go over from the conditionally positive definite case to the (strictly) positive definite case. There are different ways to define native spaces (see [10] for comparisons), but here we want to provide a technique that is general enough to unify different constructions (e.g. on the sphere [3] or on Riemannian manifolds [2],[13]). We finish

with a short account of optimal recovery of functions in native spaces from given data, and provide the corresponding error bounds based on power functions.

The notation will strictly distinguish between functions f, g, \dots and functionals λ, μ, \dots as real-valued linear maps defined on functions. Spaces of functions will be denoted by uppercase letters like F, G, \dots , and calligraphic letters $\mathcal{F}, \mathcal{G}, \dots$ occur as soon as the spaces are complete. Spaces with an asterisk are dual spaces, while an asterisk at lowercase symbols indicates optimized quantities.

2 Reproducing Kernel Hilbert Spaces

Let $\Omega \subseteq \mathbb{R}^d$ be a quite general set on which we consider real-valued functions forming a real Hilbert space \mathcal{H} with inner product $(\cdot, \cdot)_{\mathcal{H}}$. Assume further that for all $x \in \Omega$ the point evaluation functional $\delta_x : f \rightarrow f(x)$ is continuous in \mathcal{H} , i.e.

$$\delta_x \in \mathcal{H}^* \text{ for all } x \in \Omega \quad (2.1)$$

with the dual of \mathcal{H} denoted by \mathcal{H}^* . This is a reasonable assumption if we want to apply numerical methods using function values. Note, however, that techniques like the Rayleigh–Ritz method for finite elements work in Hilbert spaces where point evaluation functionals are not continuous. We shall deal with this more general situation later.

If (2.1) is satisfied, the Riesz representation theorem implies

Theorem 2.1 *If a Hilbert space of functions on Ω allows continuous point evaluation functionals, it has a symmetric reproducing kernel $\Phi : \Omega \times \Omega \rightarrow \mathbb{R}$ with the properties*

$$\begin{aligned} \Phi(x, \cdot) &\in \mathcal{H} \\ f(x) &= (f, \Phi(x, \cdot))_{\mathcal{H}} \\ \Phi(x, y) &= (\Phi(x, \cdot), \Phi(y, \cdot))_{\mathcal{H}} = \Phi(y, x) \\ \Phi(x, y) &= (\delta_x, \delta_y)_{\mathcal{H}^*} \end{aligned} \quad (2.2)$$

for all $x, y \in \Omega$, $f \in \mathcal{H}$.

The theory of reproducing kernel Hilbert spaces is well covered in [12], for instance. In the terminology following below, a reproducing kernel Hilbert space is the *native space* with respect to its reproducing kernel. This is trivial as long as we start with a Hilbert space, but it is not trivial if we start with a function $\Phi : \Omega \times \Omega \rightarrow \mathbb{R}$.

3 Invariance Properties

In many cases, the domain Ω of functions allows a group \mathbb{T} of geometric transformations, and the Hilbert space \mathcal{H} of functions on Ω is invariant under this group.

This means

$$\begin{aligned} f \circ T &\in \mathcal{H} \\ (f \circ T, g \circ T)_{\mathcal{H}} &= (f, g)_{\mathcal{H}} \end{aligned} \tag{3.1}$$

for all $f, g \in \mathcal{H}$, $T \in \mathbb{T}$. The following simple result has important implications for the basis functions on various domains:

Theorem 3.1 *If a Hilbert space \mathcal{H} of functions on a domain Ω is invariant under a group \mathbb{T} of transformations on Ω in the sense of (3.1), and if \mathcal{H} has a reproducing kernel Φ , then Φ is invariant under \mathbb{T} in the sense*

$$\Phi(x, y) = \Phi(Tx, Ty) \text{ for all } x, y \in \Omega, T \in \mathbb{T}.$$

Proof. The assertion easily follows from

$$\begin{aligned} f(x) &= (f, \Phi(x, \cdot))_{\mathcal{H}} \\ = (f \circ T^{-1})(Tx) &= (f \circ T^{-1}, \Phi(Tx, \cdot))_{\mathcal{H}} \\ &= (f \circ T^{-1} \circ T, \Phi(Tx, T \cdot))_{\mathcal{H}} \\ &= (f, \Phi(Tx, T \cdot))_{\mathcal{H}} \end{aligned}$$

for all $x \in \Omega$, $T \in \mathbb{T}$, $f \in \mathcal{H}$. ■

By some easy additional arguments one can read off the following invariance properties inherited by reproducing kernels Φ from their Hilbert spaces \mathcal{H} on Ω :

- Invariance on $\Omega = \mathbb{R}^d$ under translations from \mathbb{R}^d leads to *translation-invariant* functions $\Phi(x, y) = \phi(x - y)$ with $\phi(x) = \phi(-x) : \mathbb{R}^d \rightarrow \mathbb{R}$.
- In case of additional invariance under all orthogonal transformations we get *radial* functions $\Phi(x, y) = \phi(\|x - y\|_2)$ with $\phi : [0, \infty) \rightarrow \mathbb{R}$. Thus radial basis functions arise naturally in all Hilbert spaces on \mathbb{R}^d which are invariant under Euclidean rigid-body motions.
- Invariance on the sphere S^{d-1} under all orthogonal transformations leads to *zonal* functions $\Phi(x, y) = \phi(x^T y)$ for $\phi : [-1, 1] \rightarrow \mathbb{R}$.
- Spaces of periodic functions induce periodic reproducing kernels.

See [5] for basis functions on topological groups, and see [3] for a review of results on the sphere. The paper [13] introduces the theory of basis functions on general manifolds, and corresponding error bounds are in [2].

4 Native Spaces of Positive Definite Functions

Instead of a single point $x \in \Omega$ with a single evaluation functional $\delta_x \in \mathcal{H}^*$ we now consider a set $\{x_1, \dots, x_M\}$ of M distinct points in Ω and look at the point evaluation functionals $\delta_{x_1}, \dots, \delta_{x_M}$.

Theorem 4.1 *In a real vector space \mathcal{H} of functions on some domain Ω the following properties concerning a set $X = \{x_1, \dots, x_M\}$ of M distinct points are equivalent:*

1. *There are functions $f \in \mathcal{H}$ which attain arbitrary values at the points $x_j \in \{x_1, \dots, x_M\}$.*
2. *The points in X can be **separated**, i.e.: for all $x_j \in X$ there is a function $f_j \in \mathcal{H}$ vanishing on X except for x_j .*
3. *The point evaluation functionals $\delta_{x_1}, \dots, \delta_{x_M} \in \mathcal{H}^*$ are linearly independent.*

Now let \mathcal{H} be a reproducing kernel Hilbert space of real-valued functions on Ω . Furthermore, let one of the properties in Theorem 4.1 be satisfied for all finite sets $X = \{x_1, \dots, x_M\} \subseteq \Omega$. Then the matrix

$$A_{\Phi, X} = (\Phi(x_k, x_j))_{1 \leq j, k \leq M} = ((\delta_{x_j}, \delta_{x_k})_{\mathcal{H}^*})_{1 \leq j, k \leq M} \quad (4.1)$$

is a Gramian matrix formed of linearly independent elements. Thus it is symmetric and positive definite.

But the above property can be reformulated independent of the Hilbert space setting:

Definition 4.2 *A function $\Phi : \Omega \times \Omega \rightarrow \mathbb{R}$ is symmetric and (strictly) positive definite (SPD), if for arbitrary finite sets $X = \{x_1, \dots, x_M\} \subseteq \Omega$ of distinct points the matrix $A_{\Phi, X} = (\Phi(x_k, x_j))_{1 \leq j, k \leq M}$ is symmetric and positive definite.*

Definition 4.3 *If a symmetric (strictly) positive definite function $\Phi : \Omega \times \Omega \rightarrow \mathbb{R}$ is the reproducing kernel of a real Hilbert space \mathcal{H} of real-valued functions on Ω , then \mathcal{H} is the **native space** for Φ .*

We can collect the above arguments into

Theorem 4.4 *If a real Hilbert space \mathcal{H} of real-valued functions on some domain Ω allows continuous point evaluation functionals which are linearly independent when based on distinct points, the space has a symmetric and (strictly) positive definite reproducing kernel Φ and is the native space for Φ .*

Except for the unicity stated above, this is easy since we started from a given Hilbert space. Things are more difficult when we start with an SPD function Φ and proceed to construct its native space. The basic idea for this will first appear in the uniqueness proof for the native space:

Theorem 4.5 *The native space for a given SPD function Φ is unique if it exists, and it then coincides with the closure of the space of finite linear combinations of functions $\Phi(x, \cdot)$, $x \in \Omega$ under the inner product defined via*

$$(\Phi(x, \cdot), \Phi(y, \cdot))_{\mathcal{H}} = \Phi(x, y) \quad \text{for all } x, y \in \Omega. \quad (4.2)$$

Proof. Let \mathcal{H} be a Hilbert space of functions on Ω which has Φ as a symmetric positive definite kernel. Clearly all finite linear combinations of functions $\Phi(x, \cdot)$ are in \mathcal{H} , and the inner product on these functions depends on Φ alone because of (2.2). We can thus use (4.2) as a redefinition for the inner product on the subspace of linear combinations of functions $\Phi(x, \cdot)$. If \mathcal{H} were larger than the closure of the span of these functions, there would be a nonzero $f \in \mathcal{H}$ which is orthogonal to all $\Phi(x, \cdot)$. But then $f(x) = (f, \Phi(x, \cdot))_{\mathcal{H}} = 0$ for all $x \in \Omega$. ■

Theorem 4.5 shows that the native space is the closure of the functions we work with in applications, i.e.: the functions $\Phi(x, \cdot)$ for $x \in \Omega$ fixed. Everything that can be approximated by functions $\Phi(x, \cdot)$ is in the native space. But the above result leaves us to show existence of the native space for any SPD function Φ . To do this, we mimic (4.2) to *define* an inner product

$$(\Phi(x, \cdot), \Phi(y, \cdot))_{\Phi} = \Phi(x, y) \quad \text{for all } x, y \in \Omega. \quad (4.3)$$

on functions $\Phi(x, \cdot)$. This inner product depends on Φ alone, and we thus use a slightly different notation. It clearly extends to an inner product on the space

$$F_{\Phi}(\Omega) := \left\{ \sum_{j=1}^M \lambda_j \Phi(x_j, \cdot) \mid \lambda_j \in \mathbb{R}, M \in \mathbb{N}, x_j \in \Omega \right\} \quad (4.4)$$

of all finite linear combinations of such functions, because Φ is an SPD function. We keep Φ and Ω in the notation, because we want to study later how native spaces depend on Φ and Ω . The abstract Hilbert space completion $\mathcal{F}_{\Phi}(\Omega)$ of this space then is a Hilbert space with an inner product that we denote by $(\cdot, \cdot)_{\Phi}$ again, but we still have to interpret the abstract elements of $\mathcal{F}_{\Phi}(\Omega)$ as functions on Ω . But this is no problem since the point evaluation functionals δ_x extend continuously to the completion, and the equation

$$\delta_x(f) = (f, \Phi(x, \cdot))_{\Phi} \quad \text{for all } x \in \Omega, f \in \mathcal{F}_{\Phi}(\Omega) \quad (4.5)$$

makes sense there. We just *define* $f(x)$ to be the right-hand side of (4.5). Altogether we have

Theorem 4.6 *Any SPD function Φ on some domain Ω has a unique native space. It is the closure of the space $F_{\Phi}(\Omega)$ of (4.4) under the inner product (4.3). The elements of the native space can be interpreted as functions via (4.5).*

There are various other techniques to define the native space. See [10] for a comparison and embedding theorems.

It is one of the most challenging research topics to deduce properties of the native space from properties of Φ . For instance, Corollary 8.3 below will show that continuity of Φ on $\Omega \times \Omega$ implies that all functions in the native space are continuous on Ω . Other interesting topics are embedding theorems and density results for native spaces. See [10] for a starting point.

5 Native Spaces of Conditionally Positive Definite Functions

Several interesting functions of the form $\Phi(x, y)$ given in section 1, e.g.: Duchon's thin-plate splines or Hardy's multiquadrics are well-defined and symmetric on $\Omega = \mathbb{R}^d$ but not positive definite there. The quadratic form defined by the matrix in (4.1) is only positive definite on a certain subspace of \mathbb{R}^M . For later use, we make the corresponding precise definition somewhat more technical than necessary at first sight.

Let \mathcal{P} be a finite-dimensional subspace of real-valued functions on Ω . In applications on $\Omega \subseteq \mathbb{R}^d$ we shall usually consider $\mathcal{P} = \mathbb{P}_m^d$, the space of polynomials of order at most m , while in periodic cases we use trigonometric polynomials, or spherical harmonics on the sphere. Then $L_{\mathcal{P}}(\Omega)$ denotes the space of all linear functionals with finite support in Ω that vanish on \mathcal{P} . For convenience, we describe such functionals by the notation

$$\lambda_{X,M} : f \rightarrow \sum_{j=1}^M \lambda_j f(x_j), \quad \lambda_{X,M}(\mathcal{P}) = \{0\} \quad (5.1)$$

for finite sets $X = \{x_1, \dots, x_M\} \subseteq \Omega$ and coefficients $\lambda \in \mathbb{R}^M$. Note that these functionals form a vector space over \mathbb{R} under the usual operations.

Definition 5.1 *A function $\Phi : \Omega \times \Omega \rightarrow \mathbb{R}$ is symmetric and conditionally positive definite (CPD) with respect to \mathcal{P} , if for all $\lambda_{X,M} \in L_{\mathcal{P}}(\Omega) \setminus \{0\}$ the value of the quadratic form*

$$\sum_{j,k=1}^M \lambda_j \lambda_k \Phi(x_j, x_k) = \lambda_{X,M}^x \lambda_{X,M}^y \Phi(x, y)$$

is positive.

Here, the superscript x denotes application of the functional with respect to the variable x . The classical definition of conditional positive definiteness of some order m is related to the special case $\mathcal{P} = \mathbb{P}_m^d$ on $\Omega \subseteq \mathbb{R}^d$.

From now on we assume $\Phi : \Omega \times \Omega \rightarrow \mathbb{R}$ to be CPD with respect to a finite-dimensional space \mathcal{P} of functions on Ω . Because Φ is conditionally positive definite, we can define an inner product

$$(\lambda_{X,M}, \mu_{Y,N})_{\Phi} := \sum_{j=1}^M \sum_{k=1}^N \lambda_j \mu_k \Phi(x_j, y_k) = \lambda_{X,M}^x \mu_{Y,N}^y \Phi(x, y) \quad (5.2)$$

on the space $L_{\mathcal{P}}(\Omega)$. Furthermore, we can complete $L_{\mathcal{P}}(\Omega)$ to a Hilbert space $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$, and we denote the extended inner product on $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$ by $(\cdot, \cdot)_{\Phi}$ again. Note that $L_{\mathcal{P}}(\Omega)$ as a vector space does not depend on Φ , but the completion $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$ does, because Φ enters into the inner product. Now we can form inner products $(\lambda, \mu)_{\Phi}$ for all abstract elements λ, μ of the space $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$, but we still have no functions on Ω , because we cannot evaluate $(\lambda, \delta_x)_{\Phi}$ since δ_x is in general not in $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$.

A simple and direct, but not ultimately general workaround for this problem uses brute force to construct for all $x \in \Omega$ a substitute $\delta_{(x)} \in L_{\mathcal{P}}(\Omega)$ for a point evaluation functional. We start with the assumption of existence of a fixed set $\Xi = \{\xi_1, \dots, \xi_q\} \subseteq \Omega$ of $q = \dim \mathcal{P}$ points of Ω which is *unisolvant* for \mathcal{P} . This means that any function $p \in \mathcal{P}$ can be uniquely reconstructed from its values on Ξ . This is no serious restriction to any application. In case of classical multiquadrics or thin-plate splines in two dimensions it suffices to fix three points in Ω which are not on a line. By picking a Lagrange-type basis p_1, \dots, p_q of \mathcal{P} one can write the reconstruction as

$$p(x) = \sum_{j=1}^q p_j(x) p(\xi_j), \text{ for all } p \in \mathcal{P}, x \in \Omega. \quad (5.3)$$

This defines for all $x \in \Omega$ a very useful variation

$$\delta_{(x)}(f) := f(x) - \sum_{j=1}^q p_j(x) f(\xi_j) = \left(\delta_x - \sum_{j=1}^q p_j(x) \delta_{\xi_j} \right) (f) \quad (5.4)$$

of the standard point evaluation functional at x defined on all functions f on Ω . This functional annihilates functions from \mathcal{P} and lies in $L_{\mathcal{P}}(\Omega)$ because it is finitely supported. Furthermore, we have

$$\delta_{(\xi_j)} = 0 \text{ for the points } \xi_j \in \Xi. \quad (5.5)$$

We now can go on with our previous argument, because we can look at the function

$$R_{\Phi, \Omega}(\lambda)(x) := (\lambda, \delta_{(x)})_{\Phi}, x \in \Omega \quad (5.6)$$

which is well-defined for all abstract elements $\lambda \in \mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$. It defines a map $R_{\Phi, \Omega}$ from the abstract space $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$ into some space of functions on Ω . We have chosen

the notation $R_{\Phi,\Omega}$ because the mapping will later be continuously extended to the Riesz map on the dual of the native space. Let us look at the special situation for $\lambda = \lambda_{X,M} \in L_{\mathcal{P}}(\Omega)$. Then

$$\begin{aligned} R_{\Phi,\Omega}(\lambda_{X,M})(x) &= (\lambda_{X,M}, \delta_{(x)})_{\Phi} \\ &= \sum_{j=1}^M \lambda_j \left(\Phi(x, x_j) - \sum_{k=1}^q p_k(x) \Phi(\xi_k, x_j) \right) \\ &= \lambda_{X,M}^y \Phi(x, y) - \sum_{k=1}^q p_k(x) \lambda_{X,M}^y \Phi(\xi_k, y) \end{aligned} \quad (5.7)$$

shows the fundamental relation

$$\mu_{Y,N} R_{\Phi,\Omega}(\lambda_{X,M}) = (\lambda_{X,M}, \mu_{Y,N})_{\Phi} \quad (5.8)$$

for all $\lambda_{X,M}, \mu_{Y,N} \in L_{\mathcal{P}}(\Omega)$. It shows immediately that $R_{\Phi,\Omega}$ is injective on $L_{\mathcal{P}}(\Omega)$. We want to generalize this identity to hold on the completion $\mathcal{L}_{\Phi,\mathcal{P}}(\Omega)$, but for this we have to define a norm or inner product on the range of $R_{\Phi,\Omega}$.

This is easy, since $R_{\Phi,\Omega}$ is injective on $L_{\mathcal{P}}(\Omega)$. We can define an inner product on the range by

$$(R_{\Phi,\Omega}(\lambda), R_{\Phi,\Omega}(\mu))_{\Phi} := (\lambda, \mu)_{\Phi} \text{ for all } \lambda, \mu \in \mathcal{L}_{\Phi,\mathcal{P}}(\Omega),$$

where we extended the definition already to the completion $\mathcal{L}_{\Phi,\mathcal{P}}(\Omega)$ and used the same notation again, because we will never mix up functions with functionals here.

The space $\mathcal{F}_{\Phi,\mathcal{P}}(\Omega) := \overline{R_{\Phi,\Omega}(L_{\mathcal{P}}(\Omega))}$ for a CPD function Φ with respect to a space \mathcal{P} of functions on Ω will be the major part of the native space to be constructed. It is a Hilbert space by definition, and we have

$$R_{\Phi,\Omega} : \mathcal{L}_{\Phi,\mathcal{P}}(\Omega) := \overline{L_{\mathcal{P}}(\Omega)} \rightarrow \mathcal{F}_{\Phi,\mathcal{P}}(\Omega) \quad (5.9)$$

as the Riesz mapping and can generalize (5.8) to

$$\mu(R_{\Phi,\Omega}(\lambda)) = (R_{\Phi,\Omega}(\mu), R_{\Phi,\Omega}(\lambda))_{\Phi} = (\mu, \lambda)_{\Phi} \text{ for all } \lambda, \mu \in \mathcal{L}_{\Phi,\mathcal{P}}(\Omega) \quad (5.10)$$

by going continuously to the completions. We thus have an interpretation of the Hilbert space $\mathcal{F}_{\Phi,\mathcal{P}}(\Omega)$ as a space of functions and the Hilbert space $\mathcal{L}_{\Phi,\mathcal{P}}(\Omega)$ as a space of functionals on $\mathcal{F}_{\Phi,\mathcal{P}}(\Omega)$. Furthermore, $R_{\Phi,\Omega}$ is the Riesz map and the spaces form a dual pair.

But we still do not have a reproduction property like (2.2), and the space $\mathcal{F}_{\Phi,\mathcal{P}}(\Omega)$ has the additional and quite superficial property that all its functions vanish on Ξ due to (5.5) and (5.6). But the latter property shows that \mathcal{P} and $\mathcal{F}_{\Phi,\mathcal{P}}(\Omega)$ form a direct sum of spaces.

Definition 5.2 *The native space $\mathcal{N}_{\Phi,\mathcal{P}}(\Omega)$ for a conditionally positive definite function Φ on some domain Ω with respect to a finite-dimensional function space \mathcal{P} consists of the sum of \mathcal{P} with the Hilbert space $\mathcal{F}_{\Phi,\mathcal{P}}(\Omega)$ from (5.9).*

Note that this coincides with Definition 4.3 for $\mathcal{P} = \{0\}$, if we take Theorem 4.6 into account. To derive further properties of the native space, including a generalized notion of the reproduction equation (4.5), we use (5.3) to define a projector

$$\Pi_{\mathcal{P}}(f)(x) := \sum_{j=1}^q p_j(x) f(\xi_j) \text{ for all } f : \Omega \rightarrow \mathbb{R}, x \in \Omega$$

onto \mathcal{P} with the property that $f - \Pi_{\mathcal{P}}(f)$ always vanishes on Ξ . Thus $Id - \Pi_{\mathcal{P}}$ projects functions in the native space onto the range of $R_{\Phi, \Omega}$, i.e. on $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$. For all functions $f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ there is some $\lambda_f \in \mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$ such that we have $f - \Pi_{\mathcal{P}}f = R_{\Phi, \Omega}(\lambda_f)$, and the value of this function at some point $x \in \Omega$ is $(\lambda_f, \delta_{(x)})_{\Phi} = (R_{\Phi, \Omega}(\lambda_f), R_{\Phi, \Omega}(\delta_{(x)}))_{\Phi}$ by definition. This implies

Theorem 5.3 *Every function f in the native space of a conditionally positive definite function Φ on some domain Ω with respect to a finite-dimensional function space \mathcal{P} has the representation*

$$f(x) = (\Pi_{\mathcal{P}}f)(x) + (f - \Pi_{\mathcal{P}}f, R_{\Phi, \Omega}(\delta_{(x)}))_{\Phi} \text{ for all } x \in \Omega \quad (5.11)$$

which is a generalized Taylor-type reproduction formula.

Definition 5.4 *The dual $\mathcal{N}_{\Phi, \mathcal{P}}^*(\Omega)$ of the native space consists of all linear functionals λ defined on the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ such that the functional $\lambda - \lambda \circ \Pi_{\mathcal{P}}$ is continuous on the Hilbert subspace $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$.*

Note that the functionals $\lambda \in \mathcal{N}_{\Phi, \mathcal{P}}^*(\Omega)$ are just linear forms on $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ in the sense of linear algebra. They are not necessarily continuous on $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$ with respect to the norm $\|\cdot\|_{\Phi}$, because in that case they would have to vanish on \mathcal{P} . This would rule out point-evaluation functionals, for instance. Our special continuity requirement avoids this pitfall and makes point-evaluation functionals δ_x well-defined in the dual, but in general not continuous. However, the functional $\delta_{(x)} = \delta_x - \delta_x \circ \Pi_{\mathcal{P}}$ is continuous instead.

For all $\lambda \in \mathcal{N}_{\Phi, \mathcal{P}}^*(\Omega)$ we can consider the function $f_{\lambda} := R_{\Phi, \Omega}(\lambda - \lambda \circ \Pi_{\mathcal{P}})$ in $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$. By (5.6) and (5.2) it can be explicitly calculated via

$$\begin{aligned} f_{\lambda}(x) &= R_{\Phi, \Omega}(\lambda - \lambda \circ \Pi_{\mathcal{P}})(x) \\ &= (\lambda - \lambda \circ \Pi_{\mathcal{P}}, \delta_{(x)})_{\Phi} \\ &= (\lambda - \lambda \circ \Pi_{\mathcal{P}})^y \delta_{(x)}^z \Phi(y, z) \end{aligned} \quad (5.12)$$

By (5.8) for $f = R_{\Phi, \Omega}(\mu)$, it represents the functional λ in the sense

$$(\lambda - \lambda \circ \Pi_{\mathcal{P}})(f) = (f, f_{\lambda})_{\Phi} \text{ for all } f \in \mathcal{F}_{\Phi, \mathcal{P}}(\Omega). \quad (5.13)$$

Altogether, the action of functionals can be described by

Theorem 5.5 *Each functional λ in the dual $\mathcal{N}_{\Phi, \mathcal{P}}^*(\Omega)$ of the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ of a conditionally positive definite function Φ on some domain Ω with respect to a finite-dimensional function space \mathcal{P} acts via*

$$\begin{aligned}\lambda(f) &= (\lambda \circ \Pi_{\mathcal{P}})f + (f - \Pi_{\mathcal{P}}f, R_{\Phi, \Omega}(\lambda - \lambda \circ \Pi_{\mathcal{P}}))_{\Phi} \\ &= (\lambda \circ \Pi_{\mathcal{P}})f + (f - \Pi_{\mathcal{P}}f, \lambda^x R_{\Phi, \Omega}(\delta_{(x)}))_{\Phi}\end{aligned}$$

on all functions $f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$.

Proof. The first formula follows easily from (5.12) and (5.13). For the second, we only have to use (5.6), (5.5), and (5.8) to prove

$$\begin{aligned}\lambda^x R_{\Phi, \Omega}(\delta_{(x)})(t) &= \lambda^x R_{\Phi, \Omega}(\delta_{(t)})(x) \\ &= (\lambda - \lambda \circ \Pi_{\mathcal{P}})^x R_{\Phi, \Omega}(\delta_{(t)})(x) \\ &= (\delta_{(t)}, R_{\Phi, \Omega}(\lambda - \lambda \circ \Pi_{\mathcal{P}}))_{\Phi} \\ &= R_{\Phi, \Omega}(\lambda - \lambda \circ \Pi_{\mathcal{P}})(t) = f_{\lambda}(t)\end{aligned}\tag{5.14}$$

for all $t \in \Omega$. ■

Note how Theorem 5.5 generalizes Theorem 5.3 to arbitrary functionals from the dual of the native space. The second form is somewhat easier to apply, because the representer f_{λ} of λ can be calculated via (5.14).

6 Modified kernels

The kernel function occurring in Theorem 5.3 is by definition

$$R_{\Phi, \Omega}(\delta_{(x)})(y) = (\delta_{(x)}, \delta_{(y)})_{\Phi} =: \Psi(x, y),\tag{6.1}$$

and we call Ψ the **reduction** of Φ . It has the explicit representation

$$\begin{aligned}\Psi(x, y) &= \Phi(x, y) - \sum_{j=1}^q p_j(x) \Phi(\xi_j, y) - \sum_{k=1}^q p_k(y) \Phi(x, \xi_k) \\ &\quad + \sum_{j=1}^q \sum_{k=1}^q p_j(x) p_k(y) \Phi(\xi_j, \xi_k) \\ &= (Id - \Pi_{\mathcal{P}})^x (Id - \Pi_{\mathcal{P}})^y \Phi(x, y)\end{aligned}\tag{6.2}$$

for all $x, y \in \Omega$ because we can do the evaluation of (6.1) via (5.2) and (5.4). Furthermore, equation (6.1) implies

$$\Psi(x, y) = (R_{\Phi, \Omega} \delta_{(x)}, R_{\Phi, \Omega} \delta_{(y)})_{\Phi} = (\Psi(x, \cdot), \Psi(y, \cdot))_{\Phi}$$

as we would expect from (2.2). A consequence of (5.5) is

$$\Psi(\xi_j, \cdot) = \Psi(\cdot, \xi_j) = 0. \quad (6.3)$$

The bilinear form

$$(f, g)_\Psi := (f - \Pi_{\mathcal{P}}f, g - \Pi_{\mathcal{P}}g)_\Phi \text{ for all } f, g \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega) \quad (6.4)$$

is positive semidefinite on the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ for Φ . Its nullspace is \mathcal{P} , and the reproduction property (5.11) takes the simplified form

$$f(x) = (\Pi_{\mathcal{P}}f)(x) + (f, \Psi(x, \cdot))_\Psi \text{ for all } x \in \Omega, \quad (6.5)$$

where we used (6.3). The representer f_λ of a functional $\lambda \in \mathcal{N}_{\Phi, \mathcal{P}}^*(\Omega)$ in the sense of (5.13) takes the simplified form

$$f_\lambda(x) = \lambda^y \Psi(x, y), \quad x, y \in \Omega$$

and Theorem 5.5 goes over into

Theorem 6.1 *Each functional λ in the dual $\mathcal{N}_{\Phi, \mathcal{P}}^*(\Omega)$ of the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ of a conditionally positive definite function Φ on some domain Ω with respect to a finite-dimensional function space \mathcal{P} acts via*

$$\lambda(f) = (\lambda \circ \Pi_{\mathcal{P}})f + (f, \lambda^x \Psi(x, \cdot))_\Psi$$

on all functions $f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$.

Note that the reduction is easy to calculate. It coincides with the original function Φ if the latter is unconditionally positive definite. There also is a connection to the preconditioning technique of Jetter and Stöckler [7].

Theorem 6.2 *The reduction Ψ of Φ with respect to Ξ is (strictly) positive definite on $\Omega \setminus \Xi$.*

Proof. Let $\lambda_{X, M}$ be a functional with support $X = \{x_1, \dots, x_M\} \subseteq \Omega \setminus \Xi$. Then the functional $\lambda_{X, M}(Id - \Pi_{\mathcal{P}})$ is finitely supported on Ω and vanishes on \mathcal{P} . Thus we can use the conditional positive definiteness of Φ and get from (6.2) that

$$\lambda_{X, M}^x \lambda_{X, M}^y \Psi(x, y) = (\lambda_{X, M}(Id - \Pi_{\mathcal{P}}))^x (\lambda_{X, M}(Id - \Pi_{\mathcal{P}}))^y \Phi(x, y)$$

is nonnegative and vanishes only if $\lambda_{X, M}(Id - \Pi_{\mathcal{P}})$ is the zero functional in $L_{\mathcal{P}}(\Omega)$. Its representation is

$$\begin{aligned} \lambda_{X, M}(Id - \Pi_{\mathcal{P}})(f) &= \sum_{j=1}^M \lambda_j \left(f(x_j) - \sum_{k=1}^q p_k(x_j) f(\xi_k) \right) \\ &= \sum_{j=1}^M \lambda_j f(x_j) - \sum_{k=1}^q f(\xi_k) \sum_{j=1}^M \lambda_j p_k(x_j), \end{aligned}$$

and since the sets $X = \{x_1, \dots, x_M\}$ and Ξ are disjoint, the coefficients must vanish. ■

There is an easy possibility used in [9] to go over from here to a fully positive definite case. Using an early idea from Golomb and Weinberger [4] we form a new kernel function $K : \Omega \times \Omega \rightarrow \mathbb{R}$ by

$$K(x, y) := \Psi(x, y) + \sum_{j=1}^q p_j(x)p_j(y) \quad (6.6)$$

and a new inner product

$$(f, g)_\Phi := \sum_{j=1}^q f(\xi_j)g(\xi_j) + (f - \Pi_{\mathcal{P}}f, g - \Pi_{\mathcal{P}}g)_\Phi \quad (6.7)$$

on the whole native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$.

Theorem 6.3 *Under the new inner product (6.7) the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ for a CPD function Φ on Ω is a Hilbert space with reproducing kernel defined by (6.6). In other words $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega) = \mathcal{N}_K(\Omega)$ as vector spaces but with different though very similar topologies.*

Proof. It suffices to prove the reproduction property for some $f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ at some $x \in \Omega$ via

$$\begin{aligned} (f, K(x, \cdot))_\Phi &= \sum_{j=1}^q f(\xi_j)p_j(x) + (f - \Pi_{\mathcal{P}}f, \Psi(x, \cdot))_\Phi \\ &= (\Pi_{\mathcal{P}}f)(x) + (f - \Pi_{\mathcal{P}}f)(x) \\ &= f(x). \end{aligned}$$

Theorem 6.3 is the reason why we do not consider the CPD case to be more complicated than the SPD case. We call K the **regularized** kernel with respect to the original CPD function Φ . ■

7 Numerical treatment of modified kernels

Here, we want to describe the numerical implications induced by reduction or regularization of a kernel Φ . Consider first the standard setting of interpolation of point-evaluation data $s|_X \in \mathbb{R}^M$ in some set $X = \{x_1, \dots, x_M\} \subset \Omega$ by a CPD function Φ , where we additionally assume that point-evaluation of Φ is possible.

A generalization to Hermite–Birkhoff data will be given in section 10 below. The interpolant takes the form

$$s = p_X + R_{\Phi, \Omega}(\lambda_{X, M}), \quad p_X \in \mathcal{P}, \quad \lambda_{X, M} \in L_{\mathcal{P}}(\Omega) \quad (7.1)$$

and this gives the linear system

$$\begin{pmatrix} A_{\Phi, X} & P_X \\ P_X^T & 0 \end{pmatrix} \begin{pmatrix} \lambda \\ \rho \end{pmatrix} = \begin{pmatrix} s|_X \\ 0 \end{pmatrix}, \quad (7.2)$$

where P_X contains the values $p_j(x_k)$, $1 \leq j \leq q$, $1 \leq k \leq M$ for some arbitrary basis p_1, \dots, p_q of \mathcal{P} . The set $X = \{x_1, \dots, x_M\}$ must be \mathcal{P} -unisolvent to make the system nonsingular, and thus we can assume $\Xi \subset X$ and number the points of X such that $x_j = \xi_j$, $1 \leq j \leq q = \dim \mathcal{P}$. This induces a splitting

$$\begin{pmatrix} A_{11} & A_{12} & P_1 \\ A_{12}^T & A_{22} & P_2 \\ P_1^T & P_2^T & 0 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \rho \end{pmatrix} = \begin{pmatrix} s|_{\Xi} \\ s|_{X \setminus \Xi} \\ 0 \end{pmatrix}$$

with $q \times q$ matrices A_{11} and P_1 and an $(M - q) \times (M - q)$ matrix A_{22} . Passing to a Lagrange basis on Ξ then means setting $\sigma = P_1 \rho$ and

$$\begin{pmatrix} A_{11} & A_{12} & I \\ A_{12}^T & A_{22} & P_2 P_1^{-1} \\ I & (P_1^{-1})^T P_2^T & 0 \end{pmatrix} \begin{pmatrix} \lambda_1 \lambda_2 \\ \sigma \end{pmatrix} = \begin{pmatrix} s|_{\Xi} \\ s|_{X \setminus \Xi} \\ 0 \end{pmatrix}. \quad (7.3)$$

Now we take a closer look at the formula (6.2) and relate it to the above matrices. Denoting the identity matrix by I , we get the result

$$\begin{aligned} A_{\Psi, X} &= \begin{pmatrix} A_{11} & A_{12} \\ A_{12}^T & A_{22} \end{pmatrix} - \begin{pmatrix} I \\ P_2 P_1^{-1} \end{pmatrix} (A_{11}, A_{12}) \\ &- \begin{pmatrix} A_{11} \\ A_{12}^T \end{pmatrix} (I, (P_1^{-1})^T P_2^T) + \begin{pmatrix} I \\ P_2 P_1^{-1} \end{pmatrix} A_{11} (I, (P_1^{-1})^T P_2^T) \end{aligned}$$

and see that everything except the lower right $(M - q) \times (M - q)$ block vanishes. Setting $Y := X \setminus \Xi$ we thus have proven

$$A_{\Psi, Y} = A_{22} - P_2 P_1^{-1} A_{12} - A_{12}^T (P_1^{-1})^T P_2^T + P_2 P_1^{-1} A_{11} (P_1^{-1})^T P_2^T$$

and this matrix is symmetric and positive definite due to Theorem 6.2. If we eliminate λ_1 and σ in the system (7.3) by

$$\begin{aligned} \lambda_1 &= -(P_1^{-1})^T P_2^T \lambda_2 \\ \sigma &= s|_{\Xi} - A_{11} \lambda_1 - A_{12} \lambda_2 \\ &= s|_{\Xi} + (A_{11} (P_1^{-1})^T P_2^T - A_{12}) \lambda_2 \end{aligned} \quad (7.4)$$

we arrive at the system

$$A_{\Psi,Y}\lambda_2 = s|_Y - P_2P_1^{-1}s|_{\Xi} = s|_Y - p|_Y \quad (7.5)$$

if p is calculated beforehand from the values of s on Ξ . The algebraic reduction to the above system and the transition to the case of Theorem 6.3 take at most $\mathcal{O}(qM^2)$ operations and thus are worth while when compared to the complexity of a direct solution. Note that the transformations may spoil sparsity properties of the original matrix $A_{\Phi,X}$, but they are unnecessary anyway, if compactly supported functions on \mathbb{R}^d are used, because these are SPD, not CPD.

Finally, let us look at the numerical effect of a regularized kernel as in (6.6). Since we used a Lagrange basis of \mathcal{P} there, and since we have a special numbering, we get

$$A_{K,X} = \begin{pmatrix} I & P_Y^T \\ P_Y & A_{K,Y} \end{pmatrix}$$

with $P_Y = P_2P_1^{-1}$ and $A_{K,Y} = A_{\Psi,Y} + P_Y P_Y^T$, $A_{K,\Xi} = A_{\Psi,\Xi} + I = I$.

Note that the representation (7.1) is different from (5.11). In particular, if two interpolants s_Y , s_X based on different sets $Y \supseteq X \supseteq \Xi$ coincide on X , then necessarily $\Pi s_Y = \Pi s_X$, but not $p_X = p_Y$.

8 Properties of Native Spaces

Due to the pioneering work of Madych and Nelson [11], the native space can be written in another form. It is the largest space on which all functionals from $L_{\mathcal{P}}(\Omega)$ (and its closure $\mathcal{L}_{\Phi,\mathcal{P}}(\Omega)$) act continuously:

Theorem 8.1 *The space*

$$\mathcal{M}_{\Phi,\mathcal{P}}(\Omega) := \{f : \Omega \rightarrow \mathbb{R} : |\lambda(f)| \leq C_f \|\lambda\|_{\Phi} \text{ for all } \lambda \in L_{\mathcal{P}}(\Omega)\}$$

coincides with the native space $\mathcal{N}_{\Phi,\mathcal{P}}(\Omega)$. It has a seminorm

$$|f|_{\mathcal{M}} := \sup \{|\lambda(f)| : \lambda \in L_{\mathcal{P}}(\Omega), \|\lambda\|_{\Phi} \leq 1\} \quad (8.1)$$

which coincides with $|f|_{\Psi}$ defined via (6.4).

Proof. For all functions $f = p_f + R_{\Phi,\Omega}(\lambda_f) \in \mathcal{N}_{\Phi,\mathcal{P}}(\Omega)$ with $\lambda_f \in \mathcal{L}_{\Phi,\mathcal{P}}(\Omega)$ and $p_f \in \mathcal{P}$ we can use (5.10) to prove that f lies in the space $\mathcal{M}_{\Phi,\mathcal{P}}(\Omega)$ with $C_f \leq \|\lambda_f\|_{\Phi}$. To prove the converse, consider an arbitrary function f in $\mathcal{M}_{\Phi,\mathcal{P}}(\Omega)$ and define a functional $F_f \in L_{\mathcal{P}}(\Omega)^*$ by $F_f(\lambda) := \lambda(f)$. The definition of $\mathcal{M}_{\Phi,\mathcal{P}}(\Omega)$ makes sure that F_f is continuous on $L_{\mathcal{P}}(\Omega)$, and thus F_f can be continuously extended to $\mathcal{L}_{\Phi,\mathcal{P}}(\Omega)$. By the Riesz representation theorem, there is some $\lambda_f \in \mathcal{L}_{\Phi,\mathcal{P}}(\Omega)$ such that

$$F_f(\mu) = (\mu, \lambda_f)_{\Phi} \text{ for all } \mu \in \mathcal{L}_{\Phi,\mathcal{P}}(\Omega).$$

Then we can define the function $f - R_{\Phi, \Omega}(\lambda_f)$ and apply arbitrary functionals $\mu \in L_{\mathcal{P}}(\Omega)$ to get

$$\mu(f - R_{\Phi, \Omega}(\lambda_f)) = \mu(f) - \mu(R_{\Phi, \Omega}(\lambda_f)) = \mu(f) - (\mu, \lambda_f)_{\Phi} = \mu(f) - F_f(\mu) = 0.$$

Specializing to $\mu = \delta_{(x)}$ for all $x \in \Omega$ we see that $f - R_{\Phi, \Omega}(\lambda_f)$ coincides on Ω with a function p_f from \mathcal{P} . Thus $f = p_f + R_{\Phi, \Omega}(\lambda_f)$ is a function in the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$. This proves that the two spaces coincide as spaces of real-valued functions on Ω .

To prove the equivalence of norms, we use the above notation and first obtain $|f|_{\mathcal{M}} \leq \|\lambda_f\|_{\Phi}$ from (8.1). But since we can replace $L_{\mathcal{P}}(\Omega)$ by its closure $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$ in (8.1) and then use λ_f as a test functional, we also get

$$|f|_{\mathcal{M}} \geq |\lambda_f(f)| / \|\lambda_f\|_{\Phi} = \|\lambda_f\|_{\Phi}.$$

Due to $|f|_{\Psi} = \|\lambda_f\|_{\Phi}$ this proves the assertion. ■

We now want to give a sufficient criterion due to Mark Klein [8] for differentiability of functions in the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ of a CPD function Φ with respect to some space \mathcal{P} on $\Omega \subseteq \mathbb{R}^d$. Since this is a disguised statement about functionals in the dual space $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$, we first look at functionals:

Theorem 8.2 *Let an arbitrary functional λ be defined for functions on Ω and have the properties*

1. *The real number $\lambda^x \lambda^y \Phi(x, y)$ is well-defined and*
2. *obtainable as the “double” limit of values $\lambda_n^x \lambda_m^y \Phi(x, y)$ for a sequence $\{\lambda_k\}_k$ of finitely supported linear functionals λ_k from $L_{\mathcal{P}}(\Omega)$.*
3. *For any finitely supported linear functional $\rho \in L_{\mathcal{P}}(\Omega)$ the value $\rho^x \lambda^y \Phi(x, y)$ exists and is the limit of the values $\rho^x \lambda_n^y \Phi(x, y)$ for $n \rightarrow \infty$.*

Then the functional λ has an extension μ in the space $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$ such that all appearances of λ in the above properties can be replaced by μ . All functionals in $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$ can be obtained this way.

Proof. The second property means that for any $\epsilon > 0$ there is some $N \in \mathbb{N}$ such that

$$|\lambda^x \lambda^y \Phi(x, y) - \lambda_n^x \lambda_m^y \Phi(x, y)| < \epsilon$$

for $n, m \geq N$. Then for $c := \lambda^x \lambda^y \Phi(x, y)$ we get

$$\begin{aligned} \|\lambda_n - \lambda_m\|_{\Phi}^2 &= \|\lambda_n\|_{\Phi}^2 + \|\lambda_m\|_{\Phi}^2 - 2(\lambda_n, \lambda_m)_{\Phi} \\ &\leq \left| \|\lambda_n\|_{\Phi}^2 - c \right| + \left| \|\lambda_m\|_{\Phi}^2 - c \right| + 2|(\lambda_n, \lambda_m)_{\Phi} - c| \\ &< 4\epsilon, \end{aligned}$$

proving that $\{\lambda_k\}_k$ is a Cauchy sequence. It has a limit $\mu \in \mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$, and by continuity we have $c = (\mu, \mu)_{\Phi}$. For any finitely supported functional $\rho \in L_{\mathcal{P}}(\Omega)$ we get

$$\rho^x \lambda^y \Phi(x, y) = \lim \rho^x \lambda_n^y \Phi(x, y) = \lim (\rho, \lambda_n)_{\Phi} = (\rho, \mu)_{\Phi}.$$

Thus the action of λ on a function $R_{\Phi, \Omega}(\rho)$ coincides with the action of μ . The final statement concerning necessity of the conditions is a simple consequence of the construction of $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$. ■

The advantage of this result is that it does only involve limits of real numbers and values of finitely supported functionals (except for λ itself). A typical application is

Corollary 8.3 *Let $\Omega_1 \subseteq \Omega \subseteq \mathbb{R}^d$ be an open domain, and let derivatives of the form $(D^\alpha)^x (D^\alpha)^y \Phi(x, y)$ exist and be continuous on $\Omega_1 \times \Omega_1$ for a fixed multiindex $\alpha \in \mathbb{N}^d$. Furthermore, assume $\mathcal{P} = \mathbb{F}_m^d$ for $m < |\alpha|$ such that $D^\alpha(\mathcal{P}) = \{0\}$. Then all functions f in the native space $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$ have a continuous derivative $D^\alpha f$ on Ω_1 .*

Proof. Any pointwise multivariate derivative of order α at an interior point x can be approximated by finitely and locally supported functionals which vanish on $\mathcal{P} = \mathbb{F}_m^d$ if $m < |\alpha|$. Thus there is a functional $\delta_x^\alpha \in \mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$ which acts like this derivative on the functions in the space $R_{\Phi, \Omega}(L_{\mathcal{P}}(\Omega))$. Its action on general functions $R_{\Phi, \Omega}(\rho) \in \mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$ with $\rho \in \mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$ is also obtainable as the limit of the action of these functionals. This proves that the pointwise derivative exists for all functions in the native space.

To prove continuity of the derivative, we first evaluate

$$\begin{aligned} \|\delta_x^\alpha - \delta_y^\alpha\|_{\Phi}^2 &= \|\delta_x^\alpha\|_{\Phi}^2 + \|\delta_y^\alpha\|_{\Phi}^2 - 2(\delta_x^\alpha, \delta_y^\alpha)_{\Phi} \\ &= (D^\alpha)_{|x}^u (D^\alpha)_{|x}^v \Phi(u, v) + (D^\alpha)_{|y}^u (D^\alpha)_{|y}^v \Phi(u, v) \\ &\quad - 2(D^\alpha)_{|x}^u (D^\alpha)_{|y}^v \Phi(u, v) \end{aligned}$$

and see that the right-hand side is a continuous function. Then

$$|(D^\alpha f)(x) - (D^\alpha f)(y)|^2 = (\delta_x^\alpha - \delta_y^\alpha, R_{\Phi, \Omega}^{-1} f)_{\Phi}^2 \leq \|\delta_x^\alpha - \delta_y^\alpha\|_{\Phi}^2 \|f\|_{\Phi}^2$$

proves continuity of the derivative of functions f in the native space. ■

Lower order derivatives and more general functionals λ can be treated similarly, applying Theorem 8.2 to approximations of $\lambda - \lambda \circ \Pi_{\mathcal{P}}$.

9 Extension and Restriction

We now study the dependence of the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ on the domain. To this end, we keep the function Φ and its corresponding domain Ω fixed while looking at subdomains $\Omega_1 \subseteq \Omega$. In short,

Theorem 9.1 *Each function from a native space for a smaller domain Ω_1 contained in Ω has a canonical extension to Ω with the same seminorm, and the restriction of each function in $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ to Ω_1 lies in $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega_1)$ and has a possibly smaller norm there.*

To prove the above theorem, we have to be somewhat more precise. Consider a subset Ω_1 with

$$\Xi \subseteq \Omega_1 \subseteq \Omega \subseteq \mathbb{R}^d$$

and first extend the functionals with finite support in Ω_1 trivially to functionals on Ω . This defines a linear map

$$\epsilon_{\Omega_1} : L_{\mathcal{P}}(\Omega_1) \rightarrow L_{\mathcal{P}}(\Omega)$$

which is an isometry because the inner products are based on (5.2) in both spaces. The map extends continuously to the respective closures, and we can use the Riesz maps to define an isometric extension map

$$e_{\Omega_1} : \mathcal{F}_{\Phi, \mathcal{P}}(\Omega_1) \rightarrow \mathcal{F}_{\Phi, \mathcal{P}}(\Omega), \quad e_{\Omega_1} := R_{\Phi, \Omega} \circ \epsilon_{\Omega_1} \circ R_{\Phi, \Omega_1}^{-1}$$

between the nontrivial parts of the native spaces $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega_1)$ and $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$. The main reason behind this very general construction of canonical extensions of functions from “local” native spaces is that the variable x in (5.7) can vary in all of Ω while the support $X = \{x_1, \dots, x_M\}$ of the functional $\lambda_{X, M}$ is contained in Ω_1 . Of course, we define e_{Ω_1} on \mathcal{P} by straightforward extension of functions in \mathcal{P} , and thus have e_{Ω_1} well-defined on all of $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$.

At this point we want to mark a significant difference to the standard technique of defining local Sobolev spaces. On $\Omega = \mathbb{R}^d$ one can prove that the global Sobolev space $W_2^k(\mathbb{R}^d)$ for $k > d/2$ is the native space for the radial positive definite function

$$\Phi(x, y) = \phi(\|x - y\|_2), \quad \phi(r) = r^{k-d/2} K_{r-d/2}(r)$$

with a Bessel or Macdonald function. If we go over to localized versions of the native space, we can do this for very general (even finite) subsets Ω_1 of $\Omega = \mathbb{R}^d$, and there are no boundary effects. Furthermore, any locally defined function has a canonical extension. This is in sharp contrast to the classical construction of local Sobolev spaces, introducing functions with singularities if the boundary has incoming edges. These functions have no extension to a Sobolev space on a larger domain. Functions from local Sobolev spaces only have extensions if the domain

satisfies certain boundary conditions. Our definition always starts with the global function Φ and then does a local construction. Is our construction really “local”? To gain some more insight into this question, we have to look at the restrictions of functions from global native spaces.

Curiously enough, the restriction of functions from $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ to Ω_1 is slightly more difficult to handle than the extension. If we define $r_{\Omega_1}(f) := f|_{\Omega_1}$ for $f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$, we have to show that the result is a function in $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega_1)$.

Lemma 9.2 *The restriction map*

$$r_{\Omega_1} : \mathcal{N}_{\Phi, \mathcal{P}}(\Omega) \rightarrow \mathcal{N}_{\Phi, \mathcal{P}}(\Omega_1)$$

is well-defined and coincides with the formal adjoint of e_{Ω_1} . For any function f in $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ the “localized” seminorm $|r_{\Omega_1} f|_{\Psi, \Omega_1}$ depends only on the values of f on Ω_1 . It is a monotonic function of Ω_1 .

Proof. From the extension property of ϵ_{Ω_1} and the restriction property of r_{Ω_1} we can conclude

$$(\epsilon_{\Omega_1} \lambda_{\Omega_1})(f) = \lambda_{\Omega_1}(r_{\Omega_1} f) \text{ for all } \lambda_{\Omega_1} \in \mathcal{L}_{\Phi, \mathcal{P}}(\Omega_1), f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega). \quad (9.1)$$

This is obvious for finitely supported functionals from $L_{\mathcal{P}}(\Omega_1)$ and holds in general by continuous extension.

We use this to prove that $r_{\Omega_1}(f) := f|_{\Omega_1}$ lies in $\mathcal{M}_{\Phi, \mathcal{P}}(\Omega_1)$ for each f in $\mathcal{M}_{\Phi, \mathcal{P}}(\Omega)$. This follows from

$$|\lambda_{\Omega_1}(r_{\Omega_1} f)| = |(\epsilon_{\Omega_1} \lambda_{\Omega_1})f| \leq |f|_{\Psi, \Omega} \|\epsilon_{\Omega_1} \lambda_{\Omega_1}\|_{\Phi, \Omega} = |f|_{\Psi, \Omega} \|\lambda_{\Omega_1}\|_{\Phi, \Omega_1}$$

for all $\lambda_{\Omega_1} \in \mathcal{L}_{\Phi, \mathcal{P}}(\Omega_1)$ and all $f \in \mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$. This also proves the inequality $|r_{\Omega_1} f|_{\Psi, \Omega_1} \leq |f|_{\Psi, \Omega}$. Both inequalities are trivially satisfied for $f \in \mathcal{P}$. The monotonicity statement can be obtained by the same argument as above. Thus the norm of the restriction map is not exceeding one. Our detour via $\mathcal{M}_{\Phi, \mathcal{P}}(\Omega_1)$ implies that $|r_{\Omega_1} f|_{\Psi, \Omega_1}$ only depends on the values of f on Ω_1 . For all $f \in \mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$ and $f_{\Omega_1} \in \mathcal{F}_{\Phi, \mathcal{P}}(\Omega_1)$ equation (9.1) yields

$$\begin{aligned} (\epsilon_{\Omega_1} f_{\Omega_1}, f)_{\Phi, \Omega} &= (R_{\Phi, \Omega} \epsilon_{\Omega_1} R_{\Phi, \Omega_1}^{-1} f_{\Omega_1}, f)_{\Phi, \Omega} \\ &= (\epsilon_{\Omega_1} R_{\Phi, \Omega_1}^{-1} f_{\Omega_1})(f) \\ &= (R_{\Phi, \Omega_1}^{-1} f_{\Omega_1})(r_{\Omega_1} f) \\ &= (f_{\Omega_1}, r_{\Omega_1} f)_{\Phi, \Omega_1}. \end{aligned} \quad (9.2)$$

This is the nontrivial part of the proof that that r_{Ω_1} is the formal adjoint of e_{Ω_1} . ■

Lemma 9.3 *The above extension and restriction maps satisfy*

$$r_{\Omega_1} \circ e_{\Omega_1} = Id_{\mathcal{N}_{\Phi, \mathcal{P}}(\Omega_1)}.$$

Proof. The assertion is true on \mathcal{P} . On $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega_1)$ we use (9.2) and the fact that e_{Ω_1} is an isometry. Then for all $f_{\Omega_1}, g_{\Omega_1} \in \mathcal{F}_{\Phi, \mathcal{P}}(\Omega_1)$ we have

$$\begin{aligned} (f_{\Omega_1}, g_{\Omega_1})_{\Phi, \Omega_1} &= (e_{\Omega_1} f_{\Omega_1}, e_{\Omega_1} g_{\Omega_1})_{\Phi, \Omega} \\ &= (f_{\Omega_1}, r_{\Omega_1} e_{\Omega_1} g_{\Omega_1})_{\Phi, \Omega_1} \end{aligned}$$

Thus $g_{\Omega_1} - r_{\Omega_1} e_{\Omega_1} g_{\Omega_1}$ must be zero, because it is in $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega_1)$. ■

An interesting case of Lemma 9.2 occurs when $\Omega_1 = X = \{x_1, \dots, x_M\}$ is finite and contains Ξ . Then the functions in $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega_1)$ are of the form

$$s = p + R_{\Phi, \Omega_1}(\lambda_{X, M}), \quad p \in \mathcal{P}, \quad \lambda_{X, M} \in L_{\mathcal{P}}(\Omega_1)$$

and their seminorm is explicitly given by

$$|s|_{\Psi, \Omega_1} = \|\lambda_{X, M}\|_{\Phi}.$$

Due to Lemma 9.2 this value depends only on the values of s on $\Omega_1 = X = \{x_1, \dots, x_M\}$, and we can read off from (7.2) how this works. The value of the norm is numerically accessible. See [14] for the special case of thin-plate splines.

If we look at the extension $e_{\Omega_1} s$ of s to all of Ω we see that it has the same data on X . From

$$e_{\Omega_1}(s - \Pi_{\mathcal{P}} s) = R_{\Phi, \Omega} \epsilon_{\Omega_1} R_{\Phi, \Omega_1}^{-1}(s - \Pi_{\mathcal{P}} s)$$

$$R_{\Phi, \Omega}^{-1} e_{\Omega_1}(s - \Pi_{\mathcal{P}} s) = \epsilon_{\Omega_1} R_{\Phi, \Omega_1}^{-1}(s - \Pi_{\mathcal{P}} s)$$

one can read off that this functional has support in $X = \Omega_1$ and thus is the global form of the interpolant.

This holds also for general transfinite interpolation processes. Consider an arbitrary subset Ω_1 of Ω with $\Xi \subseteq \Omega_1$. On such a set, data are admissible if they are obtained from some function $f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$. Then $e_{\Omega_1} r_{\Omega_1} f$ has the same data on Ω_1 . Furthermore, we assert that it is the global function with least seminorm with these data. By standard arguments this boils down to proving the variational equation

$$(e_{\Omega_1} r_{\Omega_1} f, v)_{\Psi, \Omega} = 0 \quad \text{for all } v \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega) \text{ with } r_{\Omega_1} v = 0.$$

But this is trivial for $f \in \mathcal{P}$ and follows from

$$\begin{aligned} (e_{\Omega_1} r_{\Omega_1} f, v)_{\Psi, \Omega} &= (R_{\Phi, \Omega} \epsilon_{\Omega_1} R_{\Phi, \Omega_1}^{-1} r_{\Omega_1} f, v)_{\Psi, \Omega} \\ &= (\epsilon_{\Omega_1} R_{\Phi, \Omega_1}^{-1} r_{\Omega_1} f)(v) \\ &= (R_{\Phi, \Omega_1}^{-1} r_{\Omega_1} f)(r_{\Omega_1} v) \end{aligned}$$

for all $f \in \mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$. Now we can generalize a result that plays an important part in Duchon's [1] error analysis of polyharmonic splines:

Theorem 9.4 *For all functions $f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ and all subsets Ω_1 of Ω with $\Xi \subseteq \Omega_1 \subseteq \Omega$ the function $e_{\Omega_1} r_{\Omega_1} f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ has minimal seminorm in $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ under all functions coinciding with f on Ω_1 . ■*

Theorem 9.5 *The orthogonal complement of $e_{\Omega_1}(\mathcal{N}_{\Phi, \mathcal{P}}(\Omega_1))$ in $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ is the space of all functions that agree on Ω_1 with a function in \mathcal{P} .*

Proof. Use the above display again, but for $v \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ being orthogonal to all functions $g = r_{\Omega_1} f$. ■

10 Linear recovery processes

For applications of native space techniques, we want to look at general methods for reconstructing functions in the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ from given data. The data are furnished by linear functionals $\lambda_1, \dots, \lambda_N$ from $\mathcal{N}_{\Phi, \mathcal{P}}^*(\Omega)$, and the reconstruction uses functions v_1, \dots, v_N from $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$. At this point, we do not assume any link between the functionals λ_j and the functions v_j . A function $f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ is to be reconstructed via a linear quasi-interpolant

$$s_f(x) := \sum_{j=1}^N \lambda_j(f) v_j(x), \quad x \in \Omega, \quad f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$$

which should reproduce functions from \mathcal{P} by

$$p(x) = s_p(x) = \sum_{j=1}^N \lambda_j(p) v_j(x), \quad x \in \Omega, \quad p \in \mathcal{P}. \quad (10.1)$$

Then the error functional

$$\epsilon_x : f \mapsto f(x) - s_f(x), \quad \epsilon_x = \delta_x - \sum_{j=1}^N v_j(x) \lambda_j(f)$$

is in $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$ for all $x \in \Omega$ and is continuous on $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$. This setting covers a wide range of Hermite–Birkhoff interpolation or quasi-interpolation processes.

Theorem 10.1 *With the power function defined by*

$$P(x) := \|\epsilon_x\|_{\Phi}$$

the error is bounded by

$$|f(x) - s_f(x)| = |\epsilon_x(f)| \leq P(x) |f|_{\Psi} \quad \text{for all } f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega), \quad x \in \Omega.$$

Proof. Just use (10.1) and evaluate

$$\begin{aligned} |f(x) - s_f(x)| &= |\epsilon_x(f)| = |\epsilon_x(f - \Pi_{\mathcal{P}}f)| \\ &\leq \|\epsilon_x\|_{\Phi} \|f - \Pi_{\mathcal{P}}f\|_{\Phi} = P(x)|f|_{\Psi}. \end{aligned}$$

■

Theorem 10.2 *The power function can be explicitly evaluated by*

$$\begin{aligned} P^2(x) &:= \|\epsilon_x\|_{\Phi}^2 \\ &= \Psi(x, x) - 2 \sum_{j=1}^N v_j(x) \lambda_j^y \Psi(y, x) \\ &\quad + \sum_{j=1}^N \sum_{k=1}^N v_j(x) v_k(x) \lambda_j^y \lambda_k^z \Psi(y, z). \end{aligned} \tag{10.2}$$

Proof. Use

$$\epsilon_x(f) = \left(\delta_{(x)} - \sum_{j=1}^N v_j(x) \lambda_j \right) (f - \Pi_{\mathcal{P}}f)$$

for all $f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ and evaluate $\|\epsilon_x\|_{\Psi}^2 = \|\epsilon_x\|_{\Phi}^2 = P^2(x)$. ■

Note that it is in general not feasible to evaluate $\lambda^x \Phi(x, \cdot)$ for functionals $\lambda \in \mathcal{N}_{\Phi, \mathcal{P}}^*(\Omega)$ unless they are plain point evaluations or vanish on \mathcal{P} . This is why we make a detour via Ψ here and use a different representation of ϵ_x . But in many standard cases one can replace Ψ in (10.2) by Φ .

Altogether, each linear recovery process has a specific power function that describes the pointwise worst-case error for recovery of functions from the native space. The power function can be explicitly evaluated, and it would be interesting to see various examples. Now we add more information on the relation between the functionals λ_j and the functions v_j :

Theorem 10.3 *If the recovery process is interpolatory, i.e.*

$$\lambda_j(v_k) = \delta_{jk}, \quad 1 \leq j, k \leq N, \tag{10.3}$$

the error is bounded by

$$|f(x) - s_f(x)| = |\epsilon_x(f)| \leq P(x)|f - s_f|_{\Psi} \quad \text{for all } f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega), \quad x \in \Omega.$$

Furthermore, we have

$$\lambda_j(P) := \lambda_j^x \lambda_j^y (\epsilon_x, \epsilon_y)_{\Psi} = 0, \quad 1 \leq j \leq N. \tag{10.4}$$

Proof. The interpolation property implies $s_{f-s_f} = 0$, and then Theorem 10.1 can be applied to the difference $f - s_f$. This proves the error bound, and the second assertion follows directly from (10.3) when applied to (10.2) written out in two variables as required for (10.4). ■

Note that the special definition (10.4) for evaluation of $\lambda_j(P)$ is necessary because P is in general not in the native space. The new kernel function $Q(x, y) := (\epsilon_x, \epsilon_y)_\Psi$ has a form similar to the reduction of Φ . It has interesting additional properties and can in particular be used for recursive construction of interpolants and orthogonal bases. See [15] for details and [14] for a special case.

11 Optimal recovery

We now want to let the functions v_j vary freely, but we keep the functionals λ_j and the evaluation point $x \in \Omega$ fixed. Since the $v_j(x)$ influence only the power function part of the error bound, we can try to minimize the quadratic form (10.2) with respect to the N real numbers $v_j(x)$, $1 \leq j \leq N$ under the linear constraints imposed by (10.1). We do this by application of standard techniques of optimization. Picking a basis p_1, \dots, p_q of \mathcal{P} and introducing Lagrange multipliers $q_m(x)$, $1 \leq m \leq q$ for the q linear constraints from (10.1), we get that any critical point of the constrained quadratic form is a critical point of the unconstrained quadratic form

$$\begin{aligned} & \Psi(x, x) - 2 \sum_{j=1}^N v_j(x) \lambda_j^y \Psi(y, x) \\ & + \sum_{j=1}^N \sum_{k=1}^N v_j(x) v_k(x) \lambda_j^y \lambda_k^z \Psi(y, z) \\ & - 2 \sum_{m=1}^q q_m(x) \left(p_m(x) - \sum_{k=1}^N v_k(x) \lambda_k(p_m) \right) \end{aligned}$$

to be minimized with respect to the values $v_j(x)$. The equations for a critical point of the constrained quadratic form thus are

$$\begin{aligned} \lambda_k^y \Psi(x, y) &= \sum_{j=1}^N \lambda_j^y \lambda_k^z \Psi(y, z) v_j^*(x) + \sum_{m=1}^q q_m^*(x) \lambda_k(p_m) \\ p_m(x) &= \sum_{j=1}^N \lambda_j(p_m) v_j^*(x), \quad 1 \leq k \leq N, \quad 1 \leq m \leq q. \end{aligned} \tag{11.1}$$

We want to prove that this system has a unique solution. Taking a solution of the homogeneous system

$$\begin{aligned} 0 &= \sum_{j=1}^N \lambda_j^y \lambda_k^z \Psi(y, z) a_j + \sum_{m=1}^q b_m \lambda_k(p_m) \\ 0 &= \sum_{j=1}^N \lambda_j(p_m) a_j, \quad 1 \leq k \leq N, \quad 1 \leq m \leq q, \end{aligned}$$

we see that the functional

$$\chi := \sum_{j=1}^N a_j \lambda_j$$

vanishes on \mathcal{P} and thus is in $\mathcal{L}_{\Phi, \mathcal{P}}(\Omega)$. Applying it to the first N equations of (11.1) yields

$$\begin{aligned} 0 &= \sum_{j=1}^N \sum_{k=1}^N \lambda_j^y \lambda_k^z \Psi(y, z) a_j a_k + \sum_{m=1}^q b_m \sum_{k=1}^N \lambda_k(p_m) a_k \\ &= \sum_{j=1}^N \sum_{k=1}^N \lambda_j^y \lambda_k^z \Psi(y, z) a_j a_k + 0 \\ &= \chi^y \chi^z \Psi(y, z) \\ &= \chi^y \chi^z \Phi(y, z). \end{aligned}$$

Since Φ is a CPD function, we conclude that the functional χ must vanish on the native space. If we make the reasonable additional assumption that the functionals λ_j are linearly independent, we see that the coefficients a_j must vanish. This leaves us with the system

$$0 = \sum_{m=1}^q b_m \lambda_k(p_m), \quad 1 \leq k \leq N,$$

and we can conclude that all the coefficients b_m are zero, if we assume that there is no nonzero function p in \mathcal{P} for which all data $\lambda_k(p)$, $1 \leq k \leq N$ vanish.

Now we know that (11.1) has a unique solution $v_j^*(x)$, $q_m^*(x)$ for indices $1 \leq j \leq N$, $1 \leq m \leq q = \dim \mathcal{P}$. Thus the augmented unconstrained quadratic form has a unique critical point, and the same holds for the constrained quadratic form. Since the latter is nonnegative and positive definite, the critical point must be a minimum. Furthermore, we see that the optimal solution values $v_j^*(x)$, $q_m^*(x)$ are linear combinations of the right-hand values $p_m(x)$, $1 \leq m \leq q$ and $\lambda_k^y \Psi(x, y)$ for $1 \leq k \leq N$. If we apply the functional λ_j to the system, we see that the j -th column coincides with the right-hand side, and this proves that the solution must satisfy the interpolation property (10.3). Furthermore, we get $\lambda_j(q_m) = 0$ for all indices $1 \leq j \leq N$, $1 \leq m \leq q$.

But note that our solution is not just any interpolatory set of functions matching the data functionals. It is uniquely determined by the λ_j , and it is composed of functions $\lambda_j^y \Psi(y, \cdot)$ acting as the Riesz representers of the λ_j in the sense of Theorem (6.1) plus functions from \mathcal{P} . We summarize:

Theorem 11.1 *Assume that there is no nonzero function from \mathcal{P} on which all functionals λ_j vanish, and that the λ_j are linearly independent. Then the power function at any point $x \in \Omega$ can be minimized among all other power functions using the same functionals λ_j , but possibly different functions v_j . The minimum is attained for a specific set v_j^* of functions that satisfy the interpolation conditions (10.3) and are linear combinations of functions from \mathcal{P} and generalized representers of the functionals λ_j .*

We add an intrinsic characterization of the optimal power function:

Theorem 11.2 *Under the above assumptions, the optimal power function $P^*(x)$ describes the maximal value that any function $f \in \mathcal{N}_{\mathbb{F}, \mathcal{P}}(\Omega)$ can attain at $x \in \Omega$ if it satisfies the restrictions $\lambda_j(f) = 0$, $1 \leq j \leq N$ and $|f|_{\Psi} \leq 1$.*

Proof. For any such function, Theorem 10.3 implies $|f(x)| \leq P^*(x)$ because of $s_f = 0$. For fixed $x \in \Omega$, the maximal value is attained for the special function

$$f_x = \Psi(\cdot, x) - \sum_{j=1}^N v_j^*(x) \lambda_j^y \Psi(y, \cdot) - \sum_{m=1}^q q_m^*(x) p_m(\cdot)$$

after rescaling. This is due to

$$f_x(x) = (P^*(x))^2 = |f_x|_{\Psi}^2$$

which needs some elementary calculations and the identity

$$\sum_{k=1}^N v_k^*(x) \lambda_k^y \Psi(x, y) = \sum_{j=1}^N \sum_{k=1}^N v_j^*(x) v_k^*(x) \lambda_j^y \lambda_k^z \Psi(y, z) + \sum_{m=1}^q q_m^*(x) p_m(x)$$

following from (11.1). ■

Under the assumptions of Theorem 11.1 one can try to rewrite the recovery function as

$$s_f^*(x) = \sum_{j=1}^N \lambda_j^y \Psi(y, x) a_j + \sum_{m=1}^q p_m(x) b_m, \quad (11.2)$$

where the coefficients a_j satisfy

$$\sum_{j=1}^N \lambda_j(p_m) a_j = 0, \quad 1 \leq m \leq q = \dim \mathcal{P}$$

in order to form a functional from $L_{\mathcal{P}}(\Omega)$. The equations for a generalized interpolation of a function f then are

$$\begin{aligned} \lambda_k(f) = \lambda_k(s_f^*) &= \sum_{j=1}^N \lambda_j^y \lambda_k^z \Psi(y, z) a_j + \sum_{m=1}^q \lambda_k(p_m) b_m \\ 0 &= \sum_{j=1}^N \lambda_j(p_m) a_j, \quad 1 \leq k \leq N, \quad 1 \leq m \leq q, \end{aligned} \tag{11.3}$$

and the coefficient matrix coincides with the matrix in (11.1). There is much similarity to (7.2), but we are more careful here and put Ψ instead of Φ into the definition (11.2) of the recovery function, because $\lambda_j^y \Phi(y, \cdot)$ may not make sense while $\delta_{x_j}^y \Phi(y, \cdot)$ in (7.1) always is feasible.

If we take the Ψ -inner product of s_f^* with an arbitrary function g from the native space, we get

$$\begin{aligned} (s_f^*, g)_{\Psi} &= \sum_{j=1}^N a_j (\lambda_j^y \Psi(y, \cdot), g)_{\Psi} + 0 \\ &= \sum_{j=1}^N a_j \lambda_j^y (g(y) - (\Pi_{\mathcal{P}} g)(y)) \\ &= \sum_{j=1}^N a_j \lambda_j(g). \end{aligned}$$

By a standard variational argument this implies an extension of Theorem 9.4 to more general data functionals:

Theorem 11.3 *Under the hypotheses of Theorem 11.1 the function s_f^* solves the minimization problem*

$$\min \{ |g|_{\Psi} : g \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega), \lambda_j(f - g) = 0, \quad 1 \leq j \leq N \}.$$

Furthermore, the orthogonality relation

$$(f - s_f^*, s_f)_{\Psi} = 0$$

holds and implies

$$|f|_{\Psi}^2 = |f - s_f^*|_{\Psi}^2 + |s_f^*|_{\Psi}^2.$$

From section 9 we already know that the second term on the right-hand side can be calculated explicitly. The minimization principle of Theorem 11.3 implies that this value increases when more and more data functionals are used to recover the same function f . In case of reconstruction of a function from the native space, there is the upper bound $|f|_{\Psi}^2$ for these values, but for general given functions there might be no upper bound. However, the following related characterization of native spaces was proven in [16]:

Theorem 11.4 *The native space for a continuous CPD function Φ on Ω can be characterized as the set of all real-valued functions f on Ω for which there is a fixed upper bound $C_f \geq |s_f^*|_\Psi$ for all interpolants s_f^* based on arbitrary point-evaluation data $\lambda_j = \delta_{x_j}$, $x_j \in \Omega$.*

12 Connection to L_2 spaces: Overview

This section starts an analysis of native spaces directed towards the well-known representation of the “energy inner product” of classical splines in the form

$$(f, g)_\Phi = (Lf, Lg)_{L_2(\Omega)} =: (Lf, Lg) \quad (12.1)$$

with some linear differential operator L . Natural univariate splines of odd degree $2n-1$ are related to $L = d^m/dx^m$ on $\Omega = [a, b] \subset \mathbb{R}$. Furthermore, the fundamental work of Duchon on thin-plate and polyharmonic splines is based strongly on the use of $L = \Delta^m$. For general (not necessarily radial) basis functions, there is no obvious analogue of such an operator. However, we want to take advantage of (12.1) and thus proceed to work our way towards a proper definition of L .

Since the procedure is somewhat complicated, we give an overview here, and point out the reasons for certain arguments that may look like unnecessary detours. We first have to relate the native space somehow to $L_2(\Omega)$. To achieve this, we simply imbed the major part $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$ of the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega) = \mathcal{F}_{\Phi, \mathcal{P}}(\Omega) + \mathcal{P}$ into $L_2(\Omega)$. Then we study the adjoint C of the embedding, which turns out to be a convolution-type integral operator with kernel Φ that finally will be equal to $(L^*L)^{-1}$. We thus have to form the “square root” of the operator C and invert it to get L . Taking the square root requires nonnegativity of C in the sense of integral operators. This is a property that is intimately related to (strict) positive definiteness of the kernel Φ , and thus in section 16 we take a closer look at the relation of these two notions. In between, section 15 will provide a first application of the technique we develop here. In the notation we use (\cdot, \cdot) to denote the inner product in $L_2(\Omega)$.

13 Embedding into L_2

There is an easy way to imbed a native space into an L_2 space.

Lemma 13.1 *Let Φ be SPD on Ω , and let Ψ be the normalized kernel with respect to Φ as defined in section 6. Assume*

$$C_2^2 := \int_{\Omega} \Psi(x, x) dx < \infty. \quad (13.1)$$

Then the Hilbert space $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega) \subseteq \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ for Φ has a continuous linear embedding into $L_2(\Omega)$ with norm at most C_2 .

Proof: Conditional positive definiteness clearly implies that the integrand $\Psi(x, x) = (\delta_{(x)}, \delta_{(x)})_{\Phi} = \|\delta_{(x)}\|_{\Phi}^2$ is positive when forming (13.1).

Now for all $f \in \mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$ and all $x \in \Omega$ we can use the reproduction property (5.11) to get

$$\begin{aligned} f(x)^2 &= (f, \Psi(x, \cdot))_{\Phi}^2 \\ &\leq \|f\|_{\Phi}^2 \|\Psi(x, \cdot)\|_{\Phi}^2 \\ &= \|f\|_{\Phi}^2 \Psi(x, x), \end{aligned}$$

where we used $\Pi_{\mathcal{P}}f = 0$ for the functions $f \in \mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$. Then the assertion follows by integration over Ω . ■

By the way, the above inequality shows in general how upper bounds for functions in the native space can be derived from the behaviour of Ψ on the diagonal of $\Omega \times \Omega$.

14 The convolution mapping from L_2 into $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$

We now go the other way round and map $L_2(\Omega)$ into the native space.

Theorem 14.1 *Assume (13.1) to hold for a CPD function Φ on Ω . Then the integral operator*

$$C(v)(x) := \int_{\Omega} v(t) \Psi(x, t) dt \quad (14.1)$$

of generalized convolution type maps $L_2(\Omega)$ continuously into the Hilbert space $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega) \subseteq \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$. It has norm at most C_2 and satisfies

$$(f, v) = (f, C(v))_{\Phi} \text{ for all } f \in \mathcal{F}_{\Phi, \mathcal{P}}(\Omega), v \in L_2(\Omega), \quad (14.2)$$

i.e. it is the adjoint of the embedding of the Hilbert subspace $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$ of the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ into $L_2(\Omega)$.

Proof: We use the definition of $\mathcal{M}_{\Phi, \mathcal{P}}(\Omega)$ in Theorem 8.1 and pick some finitely supported functional $\lambda \in L_{\mathcal{P}}(\Omega)$ to get

$$\begin{aligned} \lambda(C(v)) &= \int_{\Omega} v(t) \lambda^x \Psi(x, t) dt \\ &\leq \|v\| \|\lambda^x \Psi(x, \cdot)\| \\ &\leq C_2 \|v\| \|\lambda\|_{\Phi} \end{aligned}$$

for all $v \in L_2(\Omega)$. In case of $f(t) := \Psi(x, t)$ with arbitrary $x \in \Omega$, equation (14.2) follows from the definition of the operator C and from the reproduction property. The general case is obtained by continuous extension. ■

Of course, equation (14.2) generalizes to

$$(f - \Pi_{\mathcal{P}}f, v) = (f - \Pi_{\mathcal{P}}f, C(v))_{\Phi} = (f, C(v))_{\Psi} \text{ for all } f \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega), v \in L_2(\Omega)$$

on the whole native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$.

We add two observations following from general properties of adjoint mappings:

Corollary 14.2 *The range of the convolution map C is dense in the Hilbert space $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$. The latter is dense in $L_2(\Omega)$ iff C is injective.*

■

Criteria for injectivity of C or, equivalently, for density of the Hilbert space $\mathcal{F}_{\Phi, \mathcal{P}}(\Omega)$ in $L_2(\Omega)$ are an open problem (in general). The main obstacle is to construct sufficiently many test functions in the native space. For classical radial basis functions on $\Omega = \mathbb{R}^d$ one can use Fourier transform techniques to prove existence of tempered or C_0^∞ test functions in the native space on \mathbb{R}^d . Then one uses the restriction technique to prove that restrictions of these functions are in the local native spaces. This is how the problem can be attacked from the global situation.

We finally remark that the above problem is related to the specific way of defining an SPD or CPD function via finitely supported functionals. Section 16 will shed some light on another feasible definition.

15 Improved convergence results

The space $C(L_2(\Omega))$ allows an improvement of the standard error estimates for reconstruction processes of functions from native spaces. Roughly speaking, the error bound can be “squared”.

Theorem 15.1 *labelTEBthree If an interpolatory recovery process in the sense of Theorem 11.1 is given, then there is a bound*

$$|f(x) - s_f^*(x)| \leq P^*(x) \|P^*\| \|v\|$$

for all $f - \Pi_{\mathcal{P}} f = C(v) \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$, $x \in \Omega$, $v \in L_2(\Omega)$. Here, we denote the optimized power function for the special situation in Theorem 11.1 by P^* .

Proof: Taking the L_2 norm of the standard error bound in 10.3, we get

$$\|f - s_f^*\| \leq \|P^*\| \|f - s_f^*\|_{\Psi}.$$

Now we use (14.2) and the orthogonality relation from Theorem 11.3:

$$\begin{aligned} \|f - s_f^*\|_{\Psi}^2 &= (f - s_f^*, f - s_f^*)_{\Psi} \\ &= (f - s_f^*, f)_{\Psi} \\ &= (f - s_f^*, C(v))_{\Psi} \\ &= (f - s_f^*, v) \\ &\leq \|f - s_f^*\| \|v\| \\ &\leq \|P^*\| \|f - s_f^*\|_{\Phi} \|v\|. \end{aligned}$$

Cancelling $\|f - s_f^*\|_\Phi$ and inserting the result into the error bound of Theorem 10.3 proves the assertion. ■

An earlier version of this result, based on Fourier transforms and restricted to functions on $\Omega = \mathbb{R}^d$ was given in [19].

16 Positive integral operators

We now look at the operator C from the point of view of integral equations. The compactness of C as an operator on $L_2(\Omega)$ will be delayed somewhat, because we first want to relate our definition of a positive definite function to that of a positive integral operator. The latter property will be crucial in later sections.

Definition 16.1 *An operator C of the form (14.1) is positive (nonnegative), if the bilinear form*

$$(w, C(v)), \quad v, w \in L_2(\Omega)$$

is symmetric and positive (nonnegative) definite on $L_2(\Omega)$.

In our special situation we can write

$$(w, C(v)) = (C(w), C(v))_\Phi, \quad v, w \in L_2(\Omega)$$

and get

Theorem 16.2 *If a symmetric and positive semidefinite function Φ on Ω satisfies (13.1), then the associated integral operator C is nonnegative. If this holds, positivity is equivalent to injectivity.*

■

Theorem 16.3 *Conversely, if C is a nonnegative integral operator of the form (13.1) with a symmetric and continuous function $\Phi : \Omega \times \Omega \rightarrow \mathbb{R}$, then Φ is positive semidefinite on Ω .*

Proof: We simply approximate point evaluation functionals δ_x by functionals on $L_2(\Omega)$ that take a local mean. Similarly, we approximate finitely supported functionals by linear combinations of the above form. The rest is standard, but requires continuity of Φ . ■

Unfortunately, the above results do not allow to conclude positive definiteness of Φ from positivity of the integral operator C . However, due to the symmetry of Φ , the integral operator C is always self-adjoint.

17 Compact nonnegative self-adjoint integral operators

To apply strong results from the theory of integral equations, we still need that C is compact on $L_2(\Omega)$. This is implied by the additional condition

$$\int_{\Omega} \int_{\Omega} \Phi(x, y)^2 dx dy < \infty \quad (17.1)$$

which is automatically satisfied if our SPD function Φ is continuous and Ω is compact. Note the difference to (13.1), which is just enough to ensure embedding of the native space into $L_2(\Omega)$.

From now on, we assume Φ to be an SPD kernel satisfying (13.1) and (17.1). Then C is a compact self-adjoint nonnegative integral operator. Now spectral theory and the theorem of Mercer [18] imply the following facts:

1. There is a finite or countable set of positive real eigenvalues $\mu_1 \geq \mu_2 \geq \dots > 0$ and eigenfunctions $\varphi_1, \varphi_2, \dots \in L_2(\Omega)$ such that

$$C(\varphi_n) = \mu_n \varphi_n, \quad n = 1, 2, \dots$$

2. The eigenvalues μ_n converge to zero for $n \rightarrow \infty$, if there are infinitely many.
3. There is an absolutely and uniformly convergent representation

$$\Phi(x, y) = \sum_n \mu_n \varphi_n(x) \varphi_n(y), \quad x, y \in \Omega.$$

4. The functions φ_n are orthonormal in $L_2(\Omega)$.
5. Together with an orthonormal basis of the kernel of C , the functions φ_n form a complete orthonormal system.
6. There is a nonnegative self-adjoint operator $\sqrt[3]{C}$ such that $C = \sqrt[3]{C} \sqrt[3]{C}$ and with an absolutely and uniformly convergent kernel representation

$$\sqrt[3]{\Phi}(x, y) := \sum_n \sqrt{\mu_n} \varphi_n(x) \varphi_n(y), \quad x, y \in \Omega,$$

where

$$\sqrt[3]{C}(v)(x) := \int_{\Omega} v(t) \sqrt[3]{\Phi}(x, t) dt, \quad x \in \Omega, \quad v \in L_2(\Omega).$$

We use the symbol $\sqrt[3]{\Phi}$ to denote the ‘‘convolution square-root’’, because

$$\Phi(x, y) = \int_{\Omega} \sqrt[3]{\Phi}(x, t) \sqrt[3]{\Phi}(t, y) dt$$

is a generalized convolution. We remark that this equation can be used for construction of new positive definite functions by convolution, and we hope to find room for details later.

The situation of finitely many eigenvalues cannot occur for the standard case of continuous SPD kernels on bounded domains with infinitely many points and linearly independent point evaluations. Otherwise, the rank of matrices of the form $(\Phi(x_j, x_k))_{1 \leq j, k \leq N}$ would have a global upper bound.

18 The native space revisited

The action of C on a general function $v \in L_2(\Omega)$ can now be rephrased as

$$C(v) = \sum_n \mu_n (v, \varphi_n) \varphi_n,$$

and it is reasonable to define an operator L such that $(L^*L)^{-1} = C$ formally by

$$L(v) = \sum_n (\mu_n)^{-1/2} (v, \varphi_n) \varphi_n. \quad (18.1)$$

We want to show that this operator nicely maps the native space into $L_2(\Omega)$, but for this we have to characterize functions from the native space in terms of expansions with respect to the functions φ_n .

Theorem 18.1 *The native space for an SPD function Φ which generates a non-negative compact integral operator on $L_2(\Omega)$ can be characterized as the space of functions $f \in L_2(\Omega)$ with $L_2(\Omega)$ -expansions*

$$f = \sum_n (f, \varphi_n) \varphi_n$$

such that the additional summability condition

$$\sum_n \frac{(f, \varphi_n)^2}{\mu_n} < \infty$$

holds.

Proof: We first show that on the subspace $C(L_2(\Omega))$ of the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ we can rewrite the inner product as

$$\begin{aligned} (C(v), C(w))_{\Phi} &= (v, C(w)) \\ &= \sum_n (v, \varphi_n) (C(w), \varphi_n) \\ &= \sum_n \frac{(C(v), \varphi_n) (C(w), \varphi_n)}{\mu_n} \end{aligned}$$

But this follows from $(C(v), \varphi_n) = \mu_n(v, \varphi_n)$ for all $v \in L_2(\Omega)$. Since $C(L_2(\Omega))$ is dense in $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ due to Corollary 14.2, and since $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ is embedded into $L_2(\Omega)$, we can rewrite the inner product on the whole native space as

$$(f, g)_{\Phi} = \sum_n \frac{(f, \varphi_n)(g, \varphi_n)}{\mu_n} \text{ for all } f, g \in \mathcal{N}_{\Phi, \mathcal{P}}(\Omega). \quad (18.2)$$

■

Corollary 18.2 *The functions $\sqrt{\mu_n}\varphi_n$ are a complete orthonormal system in the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$.*

Proof: Orthonormality immediately follows from (18.2), and Theorem 18.1 allows to rewrite all functions from the native space in the form of an orthonormal expansion

$$f = \sum_n (f, \sqrt{\mu_n}\varphi_n)_{\Phi} \sqrt{\mu_n}\varphi_n$$

with respect to the inner product of the native space. ■

Corollary 18.3 *The operator L defined in (18.1) maps the native space $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ into $L_2(\Omega)$ such that (12.1) holds. It is an isometry between its domain $\mathcal{N}_{\Phi, \mathcal{P}}(\Omega)$ and its range $L_2(\Omega)/\ker C = \text{clos}(\text{span}\{\varphi_n\}_n)$.*

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New papers added for part two:

- [18] Porter, D., and D.G. Stirling, *Integral equations: a practical treatment from spectral theory to applications*, Cambridge Texts in Applied Mathematics, Cambridge University Press 1990
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