

Error Bounds for Multiquadrics without Added Constants

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Dedicated to the memory of Professor M J D Powell FRS (1936–2015)

Abstract

While it was noted by R. Hardy and proved in a famous paper by C. A. Micchelli that radial basis function interpolants $s(x) = \sum \lambda_j \phi(\|x - \mathbf{x}_j\|)$ exist uniquely for the multiquadric radial function $\phi(r) = \sqrt{r^2 + c^2}$ as soon as the (at least two) centres are pairwise distinct, the error bounds for this interpolation problem always demanded an added constant to s . By using Pontryagin native spaces, we obtain error bounds that no longer require this additional constant expression.

1 Introduction

Among the various approaches to the approximation of continuous multivariable functions, the approximands (the continuous functions to be approximated), by simpler approximants from linear spaces, the method of radial basis functions has obtained in the last two decades a popular and successful place (Cheney and Light, 1999 [12]). Its central idea is, given a function $f : \mathbb{R}^d \rightarrow \mathbb{R}$, that is at a minimum continuous, and so-called centres $\mathbf{x}_i \in \mathbf{X} \subset \mathbb{R}^d$ which serve to define the linear space of approximants – often at the same time to place positions where approximand and approximant have to meet by means of interpolation – we use

$$s(x) = \sum_{\mathbf{x}_i \in \mathbf{X}} \lambda_{\mathbf{x}_i} K(\mathbf{x}, \mathbf{x}_i), \quad x \in \mathbb{R}^d,$$

for the approximation.

Here, in addition to the given centres, the kernel K is often defined as

$$K(\mathbf{x}, \mathbf{y}) = \phi(\|\mathbf{x} - \mathbf{y}\|)$$

with the help of a univariate, continuous function ϕ ; the latter is the radial basis function which is made multi-variate and radially symmetric by composition with

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the d -variate Euclidean norm $\|\cdot\|$. A great number of radial basis functions have turned out to be mathematically attractive and useful in several applications. A useful summary of theory and applications of radial basis functions is given for example in the book (Buhmann, 2003 [9]). For computational issues, see for instance (Beatson and Greengard, 1997 [4]).

Among them are the thin-plate splines $\phi(r) = r^2 \log r$ of (Duchon, 1979 [15]), the shifted version thereof – to avoid the removable singularity at the origin – $\phi(r) = (r^2+c^2) \log(r^2+c^2)$ (Dyn, 1987 [16]), a variety of (non-even) positive powers of r , and the famous multiquadrics and inverse multiquadrics, $\phi(r) = \sqrt{r^2+c^2}$ and its reciprocal, respectively.

One reason why these radial basis functions are so attractive is that they give rise to the aforementioned interpolation problems

$$s(\mathbf{x}_j) = f(\mathbf{x}_j), \quad \mathbf{x}_j \in \mathbf{X},$$

which turns out to be regular or even positive definite (that is, with a positive definite interpolation matrix) for several choices of radial basis functions. Among those that provide even positive definite interpolation linear systems are the inverse multiquadrics and the Gauß- and Poisson kernels ($\phi(r) = \exp(-c^2 r^2)$ and $\phi(r) = \exp(-c^2 r)$, respectively).

In all these cases, c is a positive constant. As is well known, the positive definiteness of the interpolation matrix

$$A = \{\phi(\|\mathbf{x}_i - \mathbf{x}_j\|)\}_{\mathbf{x}_i, \mathbf{x}_j \in \mathbf{X}}$$

is related to the complete monotonicity of the functions $g(t) = \phi(\sqrt{t})$ (Micchelli, 1986 [19], Powell, 1987 [20], Schoenberg, 1938 [21]).

However, we know that not all radial basis functions, and not even all of them that are mentioned in this introduction, have this property. Many of them are only conditionally positive definite because their radial part composed with the square root is not completely monotonic, but only a derivative thereof is up to a sign change and not constant. Examples are multiquadrics and (shifted) thin-plate splines which are (subject to a straightforward sign change) conditionally positive definite of order one and two, respectively. This means normally that we have to add a polynomial of that order (its degree is one less) to the approximant. The additional degrees of freedom are taken up by adding side conditions on the coefficients of this type:

$$\sum_{\mathbf{x}_i \in \mathbf{X}} \lambda_{\mathbf{x}_i} p(\mathbf{x}_i) = 0, \quad \forall p \in \Pi_k^d,$$

the notation Π_k^d being for the linear space of polynomials of order at most k in d unknowns. Due to this, one would normally add a constant (polynomial) to the multiquadrics approximant in d dimensions. However, it was noted by Micchelli (1986) [19] that this is actually not needed to guarantee the regularity of the interpolation matrix A . Therefore the question arises about the convergence estimates of such approximants without the polynomial added.

Convergence estimates, up to even spectral or exponential convergence orders to suitably smooth approximands f are readily available by Madych and Nelson

(1992) [18] for instance, for the multiquadric interpolation scheme on finitely many scattered centres with added constant and with the above mentioned side condition. See also the further papers in the same direction (Wu and Schaback, 1993 [23]), and for example (Larsson and Fornberg, 2005 [17]).

Recently, (Davydov and Schaback, 2016 [14]) have improved these classical estimates by expressing the error bounds in terms of the so-called *growth function*. These new estimates do not only imply the usual bounds in terms of the fill distance, but also allow the estimation of the consistency error of kernel-based numerical differentiation formulas. They however also require a polynomial term in the case of conditionally positive definite functions.

For infinitely many gridded data $\mathbf{X} = h\mathbb{Z}^d$, (Buhmann and Dyn, 1993 [11]) offer spectral convergence orders for multiquadrics without added constant. In this case the constant is not needed because it is exactly reproduced by the interpolant. One should also note that, when the set of centres is infinite and gridded with a positive spacing h , another approach, namely that of quasi-interpolation leads to remarkable convergence results without the addition of polynomials. One can show quite general convergence results even for approximands that are from “rougher” spaces, i.e, Sobolev spaces for instance with fewer conditions on the derivatives than the spaces the radial basis functions themselves are actually contained in. See (Buhmann and Dai, 2015 [10]) for results in great generality of this type.

It thus remains an interesting question to study the convergence orders without the polynomials added and with finitely many scattered centres. This is the aim of this work for the multiquadrics with a sign change $\phi(r) = -\sqrt{r^2 + c^2}$. It uses the fact that in case of conditionally positive definite functions of single degree we know much about their spectrum: all but one of the eigenvalues are positive and the remaining one is negative (this uses also properties of the diagonal elements which are constant $\phi(0)$, so the trace of the matrix is that times the number of centres).

A standard approach to convergence orders of radial basis functions suitably modified by added polynomials in the described manner is by the so-called *native spaces*. These are function spaces in a standard fashion defined by the generalised Fourier transforms of the radial basis functions, all of which have no zero, even if the radial basis function in question is only conditionally positive definite. When normalised to be positive, we call its radial part $\hat{\phi}$ (the [generalised] Fourier transform of a radially symmetric function even when not integrable is radially symmetric) and consider all at a minimum square-integrable approximands f to be in the native space if

$$\int_{\mathbb{R}^d} \frac{|\hat{f}(x)|^2 dx}{\hat{\phi}(\|x\|)}$$

is finite. The square-root of this expression is a semi-norm whose kernel contains the aforementioned ubiquitous polynomials. Many of the known convergence results especially for the multiquadrics radial functions are restricted to approximands from these native spaces, that is their semi-norm above has to be finite.

When these native spaces are employed, the so-called power functions are used to estimate the error of the approximants with the application of the native space semi-norm. In this paper we shall employ a related method, but we shall specif-

ically use it in the context of *Pontryagin spaces*. These are essentially the same as the most often used native spaces, except that their inner products are not just semi-inner products (that is, still non-negative), but that they are actually indefinite inner products. Concretely a Pontryagin space is a vector space with an indefinite inner product such that the maximum of the dimensions of the subspaces, where the inner product is negative for all nonzero elements, is finite. As a consequence of the aforementioned property of the interpolation matrix with a single negative eigenvalue, this is just what we need here as already noticed by (Berschneider and zu Castell, 2008 [5]), see also (Berschneider, zu Castell and Schrödl, 2012 [6]).

The crucial idea (see Lemma 2) is that the critical point of the quadratic function

$$Q(w) = K(\mathbf{z}, \mathbf{z}) - 2 \sum_{i=1}^N w_i K(\mathbf{z}, \mathbf{x}_i) + \sum_{i,j=1}^N w_i w_j K(\mathbf{x}_i, \mathbf{x}_j), \quad w \in \mathbb{R}^N,$$

which delivers the ‘weights’ associated with the kernel interpolant, coincides with the minimum of an auxiliary convex function related to a modified kernel that allows the application of the standard estimates.

The paper is organized as follows. After introducing the problem setting in Section 2 we study the properties of the quadratic function Q in Section 3 and deduce the error bounds in terms of the growth functions in Section 4 by using the results of Davydov and Schaback [14]. Finally, Section 5 is devoted to the investigation of the structure of the Pontryagin native space \mathcal{P} and its relation to the classical semi-Hilbert native space \mathcal{H} . Note that it turns out that \mathcal{H} is a subspace of \mathcal{P} with co-dimension one, in particular \mathcal{P} contains constants.

2 Preliminaries

Let $K : \Omega^2 \rightarrow \mathbb{R}$ be a continuous symmetric kernel, Ω the closure of a domain in \mathbb{R}^d , where we define $\Omega^2 := \Omega \times \Omega$. Let, furthermore, $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \Omega$ be a finite set of points such that the kernel matrix

$$K_{\mathbf{X}} := [K(\mathbf{x}_i, \mathbf{x}_j)]_{i,j=1}^N$$

is nonsingular. Then for any data vector $f = [f_1, \dots, f_N]^T \in \mathbb{R}^N$, the coefficients a_j of the K -interpolant

$$r_{\mathbf{X},K,f} = \sum_{j=1}^N a_j K(\cdot, \mathbf{x}_j) \in \mathcal{K}_{\mathbf{X}} := \text{span}\{K(\cdot, \mathbf{x}_j) : j = 1, \dots, N\}$$

are uniquely determined from the interpolation conditions

$$r_{\mathbf{X},K,f}(\mathbf{x}_i) = f_i, \quad i = 1, \dots, N.$$

This can be more easily expressed in the so-called Lagrange form. Indeed, let $u_1, \dots, u_N \in \mathcal{K}_{\mathbf{X}}$ be the Lagrange basis functions satisfying

$$u_i(\mathbf{x}_j) = \delta_{ij}, \quad \forall 1 \leq i, j \leq N,$$

where δ_{ij} is the Kronecker symbol. Clearly, in that case

$$r_{\mathbf{X},K,f}(\mathbf{x}) = \sum_{j=1}^N f_j u_j(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d.$$

We begin with

Lemma 1. *Let $\mathbf{z} \in \Omega \setminus \mathbf{X}$. The vector $w^* = [u_1(\mathbf{z}), \dots, u_N(\mathbf{z})]^T$ is a critical point of the quadratic function*

$$Q(w) = K(\mathbf{z}, \mathbf{z}) - 2w^T k_{\mathbf{z}} + w^T K_{\mathbf{X}} w, \quad w \in \mathbb{R}^N,$$

where

$$k_{\mathbf{z}} := [K(\mathbf{z}, \mathbf{x}_1), \dots, K(\mathbf{z}, \mathbf{x}_N)]^T.$$

Proof. This is a classical result which follows from the gradient of Q being zero at the vector w^* . \square

Recall that the kernel K is said to be *positive (semi-)definite* on Ω if the matrix $K_{\mathbf{X}}$ is positive (semi-)definite for any finite set $\mathbf{X} \subset \Omega$. Furthermore, K is *conditionally positive definite* on Ω with respect to a subspace $\mathcal{Q} \subset C(\Omega)$ if for any $\mathbf{X} \subset \Omega$

$$w^T K_{\mathbf{X}} w > 0$$

for all $w \in \mathbb{R}^N$, $w \neq 0$, such that

$$\sum_{i=1}^N w_i q(\mathbf{x}_i) = 0 \quad \forall q \in \mathcal{Q}.$$

In the case when $\mathcal{Q} = \Pi_k^d$, the linear space of polynomials of (total) order at most k in d unknowns, K is said to be *conditionally positive definite of order k* . In particular, K is said to be conditionally positive definite of order one if it is conditionally positive definite with respect to the space Π_1^d consisting of all constant functions.

In this paper we assume that

For any non-empty finite set $\mathbf{X} \subset \Omega$, the matrix $K_{\mathbf{X}}$ has exactly one negative eigenvalue (counted with multiplicities), and all other eigenvalues are positive. (1)

This implies in particular that $K_{\mathbf{X}}$ is non-singular and $K(\mathbf{x}, \mathbf{x}) < 0$ for all $\mathbf{x} \in \Omega$ since $K(\mathbf{x}, \mathbf{x})$ is the only eigenvalue of the matrix $K_{\{\mathbf{x}\}}$. By [5, Theorem 2] and the proof of [22, Theorem 8.5], we see that (1) is equivalent to the condition

K is conditionally positive definite with respect to a one-dimensional subspace of $C(\Omega)$, and $K(\mathbf{x}, \mathbf{x}) < 0$ for all $\mathbf{x} \in \Omega$. (2)

An example of a kernel satisfying (1) for $\Omega = \mathbb{R}^d$ is the aforementioned classical multiquadrics $K(\mathbf{x}, \mathbf{y}) = -\sqrt{\|\mathbf{x} - \mathbf{y}\|^2 + c^2}$, $c \neq 0$. Moreover, further examples are given according to [19] by the kernels of the form $K(\mathbf{x}, \mathbf{y}) = -g(\|\mathbf{x} - \mathbf{y}\|^2)$,

where $g \in C^\infty([0, \infty))$ is any function such that g' is completely monotonic but not constant and $g(0) > 0$, see e.g. [9, Theorem 2.2]. These kernels are conditionally positive definite of order one.

Any kernel K satisfying (1) is the reproducing kernel of a Pontryagin space \mathcal{P} of functions on Ω , see [1, 5]. The space \mathcal{P} can be described as follows. Let $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ be a fixed subset of Ω , and let $\lambda_1, \dots, \lambda_N$ and v_1, \dots, v_N be the eigenvalues and (real) unit (normalised) eigenvectors of $K_{\mathbf{X}}$, respectively. We assume without loss of generality that $\lambda_i > 0$, $i = 1, \dots, N-1$, and $\lambda_N < 0$. Then for

$$\psi(\mathbf{x}) := v_N^T k_{\mathbf{x}} = \sum_{j=1}^N v_{N,j} K(\mathbf{x}, \mathbf{x}_j)$$

we have

$$(\psi, \psi)_{\mathcal{P}} = v_N^T K_{\mathbf{X}} v_N = v_N^T \lambda_N v_N = \lambda_N < 0,$$

and hence $\text{span}\{\psi\}$ is a so-called *maximal negative subspace* of \mathcal{P} . This implies that the kernel

$$K^\psi(\mathbf{x}, \mathbf{y}) := K(\mathbf{x}, \mathbf{y}) - \frac{1}{\lambda_N} \psi(\mathbf{x})\psi(\mathbf{y}) \quad (3)$$

is positive semi-definite, see e.g. the proof of [1, Theorem 3.2]. Thus, K^ψ is the reproducing kernel of a Hilbert space \mathcal{H}^ψ . Then

$$\mathcal{P} = \mathcal{H}^\psi \oplus^\perp \text{span}\{\psi\}, \quad (4)$$

where \oplus^\perp denotes the orthogonal direct sum, with

$$(f + \alpha\psi, g + \beta\psi)_{\mathcal{P}} = (f, g)_{\mathcal{H}^\psi} + \lambda_N \alpha\beta, \quad f, g \in \mathcal{H}^\psi, \quad \alpha, \beta \in \mathbb{R}. \quad (5)$$

Although the splitting (4) is dependent on the choice of $\mathbf{X} \subset \mathbb{R}^d$, the space \mathcal{P} is *not*, see [1]. We call it the *Pontryagin native space* of the kernel K .

Note that

$$\mathcal{H}_0^\psi := \text{span}\{K^\psi(\cdot, \mathbf{x}) : \mathbf{x} \in \Omega\}$$

is dense in \mathcal{H}^ψ , with the inner product on \mathcal{H}_0^ψ defined by the usual formula

$$\left(\sum_{i=1}^n \alpha_i K^\psi(\cdot, \mathbf{y}_i), \sum_{j=1}^m \beta_j K^\psi(\cdot, \mathbf{z}_j) \right)_{\mathcal{H}^\psi} = \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j K^\psi(\mathbf{y}_i, \mathbf{z}_j), \quad \mathbf{y}_i, \mathbf{z}_j \in \Omega,$$

and

$$\mathcal{P}_0 := \text{span}\{K(\cdot, \mathbf{x}) : \mathbf{x} \in \Omega\}$$

is dense in \mathcal{P} , and the indefinite inner product $(\cdot, \cdot)_{\mathcal{P}}$ is given on \mathcal{P}_0 by the form

$$\left(\sum_{i=1}^n \alpha_i K(\cdot, \mathbf{y}_i), \sum_{j=1}^m \beta_j K(\cdot, \mathbf{z}_j) \right)_{\mathcal{P}} = \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j K(\mathbf{y}_i, \mathbf{z}_j), \quad \mathbf{y}_i, \mathbf{z}_j \in \Omega.$$

The density of \mathcal{P}_0 in \mathcal{P} implies by [8, Theorem B.1] that the Pontryagin native space \mathcal{P} is dense in the space of continuous functions $C(\Omega)$ with the usual maximum norm as soon as Ω is compact and $K(\mathbf{x}, \mathbf{y}) = -g(\|\mathbf{x} - \mathbf{y}\|^2)$, with $g \in C^\infty([0, \infty))$ such that $g(0) \geq 0$ and g' is strictly completely monotonic.

In the case $\mathbf{X} = \{\boldsymbol{\xi}\}$ for a single point $\boldsymbol{\xi} \in \Omega$, we have $N = 1$, $\lambda_N = K(\boldsymbol{\xi}, \boldsymbol{\xi}) < 0$ and $\psi(\mathbf{x}) = K(\mathbf{x}, \boldsymbol{\xi})$. Hence $\text{span}\{K(\cdot, \boldsymbol{\xi})\}$ is a maximal negative subspace of \mathcal{P} , and by [5, Theorem 2] we arrive at another condition equivalent to (1) and (2), namely

$$\text{For some } \boldsymbol{\xi} \in \Omega, K \text{ is conditionally positive definite with respect to } \text{span}\{K(\cdot, \boldsymbol{\xi})\}, \text{ and } K(\mathbf{x}, \mathbf{x}) < 0 \text{ for all } \mathbf{x} \in \Omega. \quad (6)$$

3 Critical point of Q

We define the auxiliary kernels

$$K^{\psi,c}(\mathbf{x}, \mathbf{y}) := K(\mathbf{x}, \mathbf{y}) - \frac{c}{\lambda_N} \psi(\mathbf{x})\psi(\mathbf{y}), \quad c > 1, \quad (7)$$

and, for a fixed $\mathbf{z} \in \Omega \setminus \mathbf{X}$, the quadratic functions

$$Q^{\psi,c}(w) = K^{\psi,c}(\mathbf{z}, \mathbf{z}) - 2w^T k_{\mathbf{z}}^{\psi,c} + w^T K_{\mathbf{X}}^{\psi,c} w,$$

with

$$K_{\mathbf{X}}^{\psi,c} := [K^{\psi,c}(\mathbf{x}_i, \mathbf{x}_j)]_{i,j=1}^N, \quad k_{\mathbf{z}}^{\psi,c} := [K^{\psi,c}(\mathbf{z}, \mathbf{x}_1), \dots, K^{\psi,c}(\mathbf{z}, \mathbf{x}_N)]^T.$$

We are now ready to formulate and prove the following key lemma.

Lemma 2. *The kernel $K^{\psi,c}$ is positive definite for any $c > 1$. Moreover,*

$$Q^{\psi,c}(w) \geq Q^{\psi,c}(w^*), \quad w \in \mathbb{R}^N,$$

where w^* is the critical point of $Q(w)$ defined in Lemma 1.

Proof. To show the first statement, we first notice that $K^{\psi,c}$ is positive semi-definite as the sum of two positive semi-definite kernels K^{ψ} and $-\frac{c-1}{\lambda_N} \psi(x)\psi(y)$. Therefore we only need to prove that $K_{\mathbf{Y}}^{\psi,c}$ is nonsingular for any finite set $\mathbf{Y} = \{\mathbf{y}_1, \dots, \mathbf{y}_M\} \subset \Omega$. Assume that $K_{\mathbf{Y}}^{\psi,c} v = 0$ for some $v \in \mathbb{R}^M$. Then

$$0 = v^T K_{\mathbf{Y}}^{\psi,c} v = v^T K_{\mathbf{Y}}^{\psi} v - \frac{c-1}{\lambda_N} \left(\sum_{j=1}^M v_j \psi(y_j) \right)^2 \geq -\frac{c-1}{\lambda_N} \left(\sum_{j=1}^M v_j \psi(y_j) \right)^2,$$

which implies

$$\sum_{j=1}^M v_j \psi(y_j) = 0.$$

Hence

$$K_{\mathbf{Y}} v = K_{\mathbf{Y}}^{\psi,c} v + \frac{c}{\lambda_N} [\psi(\mathbf{y}_1), \dots, \psi(\mathbf{y}_M)]^T \sum_{j=1}^M v_j \psi(y_j) = 0,$$

and since $K_{\mathbf{Y}}$ is nonsingular in view of (1), it follows that $v = 0$.

Furthermore, let

$$D := \text{diag}(\lambda_1, \dots, \lambda_N) = V K_{\mathbf{X}} V^T,$$

where $V := [v_1, \dots, v_N]^T$. Then

$$Q(w) = K(\mathbf{z}, \mathbf{z}) - 2\bar{w}^T a + \bar{w}^T D \bar{w}, \quad a := V k_{\mathbf{z}}, \quad \bar{w} := V w.$$

Hence

$$\begin{aligned} Q(w) &= K(\mathbf{z}, \mathbf{z}) - 2 \sum_{i=1}^N a_i \bar{w}_i + \sum_{i=1}^N \lambda_i \bar{w}_i^2 \\ &= K(\mathbf{z}, \mathbf{z}) - \sum_{i=1}^N \frac{a_i^2}{\lambda_i} + \sum_{i=1}^N \lambda_i \left(\bar{w}_i - \frac{a_i}{\lambda_i} \right)^2, \end{aligned}$$

with

$$a_i = v_i^T k_{\mathbf{z}} = \sum_{j=1}^N v_{ij} K(\mathbf{z}, \mathbf{x}_j).$$

In particular,

$$a_N = \psi(\mathbf{z}).$$

This shows that the (only) critical point $w^* = V^T \bar{w}^*$ of Q satisfies

$$\bar{w}_i^* = \frac{a_i}{\lambda_i}, \quad i = 1, \dots, N.$$

Therefore, w^* is also a critical point and indeed the minimum of the strictly convex quadratic function

$$\bar{Q}(w) = Q(w) - c \lambda_N \left(\bar{w}_N - \frac{a_N}{\lambda_N} \right)^2.$$

We now show that $\bar{Q}(w)$ coincides with $Q^{\psi, c}(w)$. Indeed,

$$v_N = \lambda_N^{-1} K_{\mathbf{X}} v_N = \lambda_N^{-1} [\psi(\mathbf{x}_1), \dots, \psi(\mathbf{x}_N)]^T,$$

and hence

$$v_N v_N^T = \lambda_N^{-2} [\psi(\mathbf{x}_i) \psi(\mathbf{x}_j)]_{i,j=1}^N.$$

Thus,

$$\begin{aligned} \bar{Q}(w) &= Q(w) - c \left(\frac{a_N^2}{\lambda_N} - 2a_N \bar{w}_N + \lambda_N \bar{w}_N^2 \right) \\ &= Q(w) - c \left(\frac{\psi(\mathbf{z})^2}{\lambda_N} - 2\psi(\mathbf{z}) w^T v_N + \lambda_N w^T v_N v_N^T w \right) \\ &= Q(w) - \frac{c}{\lambda_N} \left(\psi(\mathbf{z})^2 - 2w^T \psi(\mathbf{z}) [\psi(\mathbf{x}_1), \dots, \psi(\mathbf{x}_N)]^T + w^T [\psi(\mathbf{x}_i) \psi(\mathbf{x}_j)]_{i,j=1}^N w \right) \\ &= Q^{\psi, c}(w). \end{aligned}$$

This completes the proof of the second statement of the lemma. \square

This leads to an error bound in terms of $Q^{\psi, c}(w^*)$.

Lemma 3. *Let $f \in \mathcal{P}$. Then for any $c > 1$*

$$|f(\mathbf{z}) - r_{\mathbf{X},K,f}(\mathbf{z})|^2 \leq Q^{\psi,c}(w^*) \left((f, f)_{\mathcal{P}} + \frac{1}{|\lambda_N|} \sum_{j=1}^N |f(\mathbf{x}_j)|^2 \right).$$

Proof. Let

$$f = f^+ + \gamma\psi, \quad f^+ \in \mathcal{H}^\psi, \quad \gamma \in \mathbb{R}.$$

Then

$$\gamma = \frac{(f, \psi)_{\mathcal{P}}}{(\psi, \psi)_{\mathcal{P}}} = \lambda_N^{-1} \sum_{j=1}^N v_{N,j} (f, K(\cdot, \mathbf{x}_j))_{\mathcal{P}} = \lambda_N^{-1} \sum_{j=1}^N v_{N,j} f(\mathbf{x}_j),$$

and hence

$$(f, f)_{\mathcal{P}} = (f^+, f^+)_{\mathcal{P}} + \gamma^2 (\psi, \psi)_{\mathcal{P}} = \|f^+\|_{\mathcal{H}^\psi}^2 + \lambda_N^{-1} \left(\sum_{j=1}^N v_{N,j} f(\mathbf{x}_j) \right)^2,$$

which implies by the normalisation of the eigenvector

$$\|f^+\|_{\mathcal{H}^\psi}^2 \leq (f, f)_{\mathcal{P}} - \lambda_N^{-1} \sum_{j=1}^N |f(\mathbf{x}_j)|^2 = (f, f)_{\mathcal{P}} + \frac{1}{|\lambda_N|} \sum_{j=1}^N |f(\mathbf{x}_j)|^2. \quad (8)$$

Since $\psi \in \mathcal{K}_{\mathbf{X}}$, we have $r_{\mathbf{X},K,\psi}(\mathbf{z}) = \psi(\mathbf{z})$. Hence by Lemmas 1 and 2,

$$\begin{aligned} f(\mathbf{z}) - r_{\mathbf{X},K,f}(\mathbf{z}) &= f^+(\mathbf{z}) - \sum_{j=1}^N f_j^+ u_j(\mathbf{z}) \\ &= f^+(\mathbf{z}) - \sum_{j=1}^N f_j^+ w_j^* \\ &= f^+(\mathbf{z}) - r_{\mathbf{X},K^{\psi,c},f^+}(\mathbf{z}), \end{aligned}$$

for any $c > 1$. By the standard estimate for the kernel interpolation error in terms of the power function, see e.g. [22, Theorem 11.4], we obtain

$$|f^+(\mathbf{z}) - r_{\mathbf{X},K^{\psi,c},f^+}(\mathbf{z})| \leq \sqrt{Q^{\psi,c}(w^*)} \|f^+\|_{\mathcal{H}^{\psi,c}}, \quad (9)$$

where $\mathcal{H}^{\psi,c}$ is the native space of the kernel $K^{\psi,c}$, that is the Hilbert space of continuous functions on Ω , for which $K^{\psi,c}$ is the reproducing kernel. Since $K^{\psi,c} - K^\psi$ is a positive semi-definite kernel, we have

$$\|f^+\|_{\mathcal{H}^{\psi,c}} \leq \|f^+\|_{\mathcal{H}^\psi},$$

see [2, Section 7], and the lemma follows from (9) and (8). \square

4 Error bounds

We now prove a bound on $Q^{\psi,c}(w^*)$ in terms of the *growth function* $\rho_q(\mathbf{z}, \mathbf{X})$ defined by

$$\rho_q(\mathbf{z}, \mathbf{X}) = \sup \{p(\mathbf{z}) : p \in \Pi_q^d, |p(\mathbf{x}_i)| \leq \|\mathbf{x}_i - \mathbf{z}\|_2^q, i = 1, \dots, N\}, \quad (10)$$

see [13, 3, 14]. We will use the following notation for the partial derivatives of the kernel K distinguishing its both d -dimensional arguments:

$$\partial^{\alpha,\beta} K(\mathbf{x}, \mathbf{y}) := \frac{\partial^{|\alpha|}}{\partial \mathbf{x}^\alpha} \left(\frac{\partial^{|\beta|}}{\partial \mathbf{y}^\beta} K(\mathbf{x}, \mathbf{y}) \right),$$

where

$$\partial^\alpha := \frac{\partial^{|\alpha|}}{\partial \mathbf{x}^\alpha} = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \dots \partial x_d^{\alpha_d}}, \quad |\alpha| = \alpha_1 + \dots + \alpha_d, \quad \alpha \in \mathbb{Z}_+^d,$$

as well as the usual abbreviations

$$\alpha! = \alpha_1! \dots \alpha_d!, \quad \binom{|\alpha|}{\alpha} := \frac{|\alpha|!}{\alpha!}.$$

Lemma 4. *Assume that $S_{\mathbf{z}, \mathbf{X}} := \cup_{i=1}^N [\mathbf{z}, \mathbf{x}_i] \subset \Omega$. Let $q \geq 1$ be such that*

$$\partial^{\alpha,\beta} K \in C(\Omega^2), \quad \text{for all } |\alpha|, |\beta| \leq q. \quad (11)$$

Then for any $c > 1$,

$$Q^{\psi,c}(w^*) \leq \rho_q^2(\mathbf{z}, \mathbf{X}) \frac{1}{(q!)^2} \left(M_q(K) + \frac{Nc}{|\lambda_N|} \mu_q(K) \right), \quad (12)$$

where

$$M_q(K) := \left(\sum_{|\alpha|, |\beta|=q} \binom{q}{\alpha} \binom{q}{\beta} \|\partial^{\alpha,\beta} K\|_{C(\Omega^2)}^2 \right)^{1/2},$$

$$\mu_q(K) := \sum_{|\alpha|=q} \binom{q}{\alpha} \|\partial^{\alpha,0} K\|_{C(\Omega^2)}^2.$$

Proof. In view of Lemma 2, we obtain by [14, Theorem 9],

$$Q^{\psi,c}(w^*) \leq \rho_q^2(\mathbf{z}, \mathbf{X}) \frac{M_q(K^{\psi,c})}{(q!)^2}.$$

Since

$$\begin{aligned} |\partial^{\alpha,\beta}(\psi(\mathbf{x})\psi(\mathbf{y}))| &= \left| \sum_{i=1}^N v_{N,i} \partial^{\alpha,0} K(\mathbf{x}, \mathbf{x}_i) \sum_{j=1}^N v_{N,j} \partial^{\beta,0} K(\mathbf{y}, \mathbf{x}_j) \right| \\ &\leq \left(\sum_{i=1}^N \left(\partial^{\alpha,0} K(\mathbf{x}, \mathbf{x}_i) \right)^2 \right)^{1/2} \left(\sum_{j=1}^N \left(\partial^{\beta,0} K(\mathbf{y}, \mathbf{x}_j) \right)^2 \right)^{1/2} \\ &\leq N \max_{1 \leq i \leq N} |\partial^{\alpha,0} K(\mathbf{x}, \mathbf{x}_i)| \max_{1 \leq i \leq N} |\partial^{\beta,0} K(\mathbf{y}, \mathbf{x}_i)|, \end{aligned}$$

it follows by the definition of $K^{\psi,c}$ that

$$\|\partial^{\alpha,\beta} K^{\psi,c}\|_{C(\Omega^2)} \leq \|\partial^{\alpha,\beta} K\|_{C(\Omega^2)} + \frac{Nc}{|\lambda_N|} \|\partial^{\alpha,0} K\|_{C(\Omega^2)} \|\partial^{\beta,0} K\|_{C(\Omega^2)},$$

which implies

$$\begin{aligned} M_q(K^{\psi,c}) &\leq M_q(K) + \frac{Nc}{|\lambda_N|} \left(\sum_{|\alpha|,|\beta|=q} \binom{q}{\alpha} \binom{q}{\beta} \|\partial^{\alpha,0} K\|_{C(\Omega^2)}^2 \|\partial^{\beta,0} K\|_{C(\Omega^2)}^2 \right)^{1/2} \\ &= M_q(K) + \frac{Nc}{|\lambda_N|} \sum_{|\alpha|=q} \binom{q}{\alpha} \|\partial^{\alpha,0} K\|_{C(\Omega^2)}^2. \end{aligned}$$

□

It follows from (1) with $\mathbf{X} = \{\mathbf{x}\}$ that $K(\mathbf{x}, \mathbf{x})$ is negative for any $\mathbf{x} \in \Omega$.

Lemma 5. *Assume that $K(\mathbf{x}_i, \mathbf{x}_i) \leq \varkappa < 0$ for all $i = 1, \dots, N$. Then $|\lambda_N| \geq N|\varkappa|$.*

Proof. Indeed, the trace of $K_{\mathbf{X}}$ is less or equal to $N\varkappa < 0$. Since λ_N is the only negative eigenvalue of $K_{\mathbf{X}}$, it follows that $\lambda_N \leq -\sum_{i=1}^{N-1} \lambda_i + N\varkappa \leq N\varkappa$. □

Our main error bound now follows in the theorem

Theorem 6. *Assume that $K : \Omega^2 \rightarrow \mathbb{R}$ is a continuous symmetric kernel satisfying (1). We assume in addition that $K(\mathbf{x}, \mathbf{x}) \leq -1$ for all $\mathbf{x} \in \Omega$ and denote by \mathcal{P} the native Pontryagin space of K . Let $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \Omega$ and $\mathbf{z} \in \Omega$ be such that $\cup_{i=1}^N [\mathbf{z}, \mathbf{x}_i] \subset \Omega$. Then for any $f \in \mathcal{P}$ and any $q \geq 1$ such that $\partial^{\alpha,\beta} K \in C(\Omega^2)$ for all $|\alpha|, |\beta| \leq q$,*

$$|f(\mathbf{z}) - r_{\mathbf{X},K,f}(\mathbf{z})| \leq \rho_q(\mathbf{z}, \mathbf{X}) \tilde{M}_q(K) \left((f, f)_{\mathcal{P}} + \frac{1}{N} \sum_{j=1}^N |f(\mathbf{x}_j)|^2 \right)^{1/2}, \quad (13)$$

where $\tilde{M}_q(K) = (M_q(K) + \mu_q(K))^{1/2}/q!$.

Proof. By combining Lemmas 3 and 4 we obtain for any $c > 1$ the estimate that

$$\begin{aligned} &|f(\mathbf{z}) - r_{\mathbf{X},K,f}(\mathbf{z})| \leq \\ &\leq \rho_q(\mathbf{z}, \mathbf{X}) \frac{1}{q!} \left(M_q(K) + \frac{Nc}{|\lambda_N|} \mu_q(K) \right)^{1/2} \left((f, f)_{\mathcal{P}} + \frac{1}{|\lambda_N|} \sum_{j=1}^N |f(\mathbf{x}_j)|^2 \right)^{1/2}. \end{aligned}$$

By letting $c \rightarrow 1$ and using Lemma 5 with $\varkappa = -1$, we obtain (13). □

It is easy to check that applying Lemmas 3–5 to a kernel $K(\mathbf{x}, \mathbf{y})$ satisfying

$$\varkappa = \sup_{\mathbf{x} \in \Omega} K(\mathbf{x}, \mathbf{x}) < 0 \quad (14)$$

results in exactly the same interpolation method and the same estimate as obtained from Theorem 6 for the kernel $K'(\mathbf{x}, \mathbf{y}) := K(\mathbf{x}, \mathbf{y})/|\varkappa|$. Indeed, this follows from the fact that $M_q(K') = M_q(K)/|\varkappa|$, $\mu_q(K') = \mu_q(K)/|\varkappa|^2$ and $(f, g)_{\mathcal{P}'} = |\varkappa|(f, g)_{\mathcal{P}}$, where \mathcal{P}' is the native Pontryagin space of K' . Hence there is no loss of generality in assuming that $K(\mathbf{x}, \mathbf{x}) \leq -1$ rather than (14).

5 Relation between two types of native spaces

We now assume that the kernel K satisfies (1) and is conditionally positive definite of order one. We recall the standard construction of a semi-Hilbert reproducing kernel space \mathcal{H} usually referred to as the native space of such a kernel K , see e.g. [22, Section 10.3].

Fix a point $\boldsymbol{\xi} \in \Omega$ and consider the kernel

$$K^\xi(\mathbf{x}, \mathbf{y}) := K(\mathbf{x}, \mathbf{y}) - K(\boldsymbol{\xi}, \mathbf{y}) - K(\mathbf{x}, \boldsymbol{\xi}) + K(\boldsymbol{\xi}, \boldsymbol{\xi}).$$

It is easy to see that this kernel is positive definite as soon as K is conditionally positive definite of order one. The *semi-Hilbert native space* associated with K can be described as

$$\mathcal{H} = \mathcal{H}^\xi \oplus^\perp \Pi_1^d,$$

where \mathcal{H}^ξ is the reproducing kernel Hilbert space with kernel K^ξ , and the inner product of \mathcal{H} is defined to be zero on the space of constants. As $K^\xi(\boldsymbol{\xi}, \mathbf{x}) = 0$, it is clear that

$$\mathcal{H}^\xi = \{f \in \mathcal{H} : f(\boldsymbol{\xi}) = 0\}.$$

For a fixed $\boldsymbol{\xi}$ we may also consider the kernel K^ψ defined by (3) in the special case of $\mathbf{X} = \{\boldsymbol{\xi}\}$. In this case $N = 1$, the only eigenvalue of $K_{\mathbf{X}}$ is $\lambda_N = K(\boldsymbol{\xi}, \boldsymbol{\xi}) < 0$ in view of (1), and $\psi(\mathbf{x}) = K(\mathbf{x}, \boldsymbol{\xi})$, so that K^ψ becomes

$$\tilde{K}^\xi(\mathbf{x}, \mathbf{y}) := K(\mathbf{x}, \mathbf{y}) - \frac{1}{K(\boldsymbol{\xi}, \boldsymbol{\xi})} K(\mathbf{x}, \boldsymbol{\xi}) K(\boldsymbol{\xi}, \mathbf{y}).$$

It follows from (4) that

$$\mathcal{P} = \tilde{\mathcal{H}}^\xi \oplus^\perp \text{span}\{K(\cdot, \boldsymbol{\xi})\},$$

where $\tilde{\mathcal{H}}^\xi \subset \mathcal{P}$ is the Hilbert space for which \tilde{K}^ξ is the reproducing kernel. Since $\tilde{K}^\xi(\boldsymbol{\xi}, \mathbf{y}) = 0$ and $K(\boldsymbol{\xi}, \boldsymbol{\xi}) \neq 0$, it follows that

$$\tilde{\mathcal{H}}^\xi = \{f \in \mathcal{P} : f(\boldsymbol{\xi}) = 0\},$$

which shows that $\tilde{\mathcal{H}}^\xi$ plays for \mathcal{P} a role similar to the role \mathcal{H}^ξ plays for \mathcal{H} .

It turns out that \mathcal{H}^ξ is a subspace of $\tilde{\mathcal{H}}^\xi$ of codimension one. Indeed, it is easy to see that

$$\tilde{K}^\xi(\mathbf{x}, \mathbf{y}) - K^\xi(\mathbf{x}, \mathbf{y}) = -\frac{w_\xi(\mathbf{x})w_\xi(\mathbf{y})}{K(\boldsymbol{\xi}, \boldsymbol{\xi})}, \quad w_\xi := K(\cdot, \boldsymbol{\xi}) - K(\boldsymbol{\xi}, \boldsymbol{\xi}).$$

By [2, §3], $\tilde{K}^\xi - K^\xi$ is the positive semi-definite reproducing kernel of the one-dimensional Hilbert space $\text{span}\{w_\xi\}$, with the inner product

$$(\alpha w_\xi, \beta w_\xi) = -K(\boldsymbol{\xi}, \boldsymbol{\xi})\alpha\beta, \quad \alpha, \beta \in \mathbb{R}.$$

By [2, §6], $\tilde{\mathcal{H}}^\xi = \mathcal{H}^\xi + \text{span}\{w_\xi\}$, and since $\tilde{K}^\xi - K^\xi \neq 0$ it follows that this is an orthogonal direct sum, which proves the following lemma.

Lemma 7. For any $\xi \in \Omega$,

$$\tilde{\mathcal{H}}^\xi = \mathcal{H}^\xi \oplus^\perp \text{span}\{w_\xi\},$$

and

$$(f + \alpha w_\xi, g + \beta w_\xi)_\mathcal{P} = (f, g)_\mathcal{H} - \alpha\beta K(\xi, \xi), \quad f, g \in \mathcal{H}^\xi, \quad \alpha, \beta \in \mathbb{R}.$$

By (4) and (5) it now follows that

$$\mathcal{P} = \mathcal{H}^\xi \oplus^\perp \text{span}\{w_\xi\} \oplus^\perp \text{span}\{K(\cdot, \xi)\}, \quad (15)$$

and for all $f, g \in \mathcal{H}^\xi$ and $\alpha, \beta, \gamma, \delta \in \mathbb{R}$,

$$(f + \alpha w_\xi + \gamma K(\cdot, \xi), g + \beta w_\xi + \delta K(\cdot, \xi))_\mathcal{P} = (f, g)_\mathcal{H} - (\alpha\beta - \gamma\delta)K(\xi, \xi). \quad (16)$$

We deduce the following result that clarifies the relation between \mathcal{P} and \mathcal{H} .

Theorem 8. Assume that the kernel K satisfies (1) and is conditionally positive definite of order one on Ω . Then for any $\xi \in \Omega$,

$$\mathcal{P} = \mathcal{H} \oplus \text{span}\{K(\cdot, \xi)\}, \quad (17)$$

and for all $f, g \in \mathcal{H}$ and $\alpha, \beta \in \mathbb{R}$,

$$(f + \alpha K(\cdot, \xi), g + \beta K(\cdot, \xi))_\mathcal{P} = (f, g)_\mathcal{H} + \beta f(\xi) + \alpha g(\xi) + \alpha\beta K(\xi, \xi). \quad (18)$$

Proof. The first statement follows from (15) since

$$\text{span}\{w_\xi\} \oplus^\perp \text{span}\{K(\cdot, \xi)\} = \Pi_1^d \oplus \text{span}\{K(\cdot, \xi)\}$$

and $\mathcal{H} = \mathcal{H}^\xi \oplus^\perp \Pi_1^d$. To prove (18) we recall that K is the reproducing kernel of \mathcal{P} , which implies $(f, K(\cdot, \xi))_\mathcal{P} = f(\xi)$, $(g, K(\cdot, \xi))_\mathcal{P} = g(\xi)$ and $(K(\cdot, \xi), K(\cdot, \xi))_\mathcal{P} = K(\xi, \xi)$. \square

Note that the direct sum in (17) is *not* orthogonal. We now summarize some further properties of \mathcal{H}, \mathcal{P} .

Proposition 9. $\Pi_1^d \subset \mathcal{H} \subset \mathcal{P}$. Moreover,

$$(f, g)_\mathcal{P} = (f, g)_\mathcal{H} \quad \text{for all } f, g \in \mathcal{H}, \quad (19)$$

$$(p, p)_\mathcal{P} = 0 \quad \text{for all } p \in \Pi_1^d \quad (20)$$

$$\mathcal{H}^\perp = \Pi_1^d. \quad (21)$$

Proof. The first statement and (19) are immediate consequences of Theorem 8, whereas (20) is a special case of (19), or it can be obtained from (16) since

$$1 = \alpha w_\xi - \alpha K(\cdot, \xi), \quad \text{with } \alpha = -\frac{1}{K(\xi, \xi)}.$$

Let $f \in \mathcal{H} = \mathcal{H}^\xi \oplus^\perp \Pi_1^d$. Then f has a unique representation

$$f = f^\xi + \alpha w_\xi - \alpha K(\cdot, \xi), \quad \text{for some } f^\xi \in \mathcal{H}^\xi, \alpha \in \mathbb{R}.$$

Hence, by (16), for any $g = g^\xi + \beta w_\xi + \delta K(\cdot, \xi) \in \mathcal{P}$, with $g^\xi \in \mathcal{H}^\xi$, we have

$$(f, g)_\mathcal{P} = (f^\xi, g^\xi)_\mathcal{H} - K(\xi, \xi)\alpha(\beta + \delta),$$

and

$$g \in \mathcal{H}^\perp := \{g \in \mathcal{P} : (f, g)_\mathcal{P} = 0, \quad \forall f \in \mathcal{H}\}$$

if and only if $g^\xi = 0$ and $\beta + \delta = 0$, that is $g = \delta K(\xi, \xi) \in \Pi_1^d$. \square

In the terminology of the theory of indefinite inner product spaces, see [7], (21) implies that \mathcal{H} is a *degenerate subspace* of \mathcal{P} as its *isotropic part* $\mathcal{H} \cap \mathcal{H}^\perp = \Pi_1^d$ is nontrivial. In particular, (17) cannot be replaced by an orthogonal direct sum with \mathcal{H} as a factor.

In the case when K is translation-invariant and $\Omega = \mathbb{R}^d$ we can use Theorem 8 and [22, Theorem 10.21] to establish a full description of the Pontryagin native space \mathcal{P} via Fourier transforms.

Theorem 10. *Let K be a continuous symmetric translation-invariant kernel*

$$K(\mathbf{x}, \mathbf{y}) = \Phi(\mathbf{x} - \mathbf{y}),$$

which is conditionally positive definite of order one on \mathbb{R}^d . Assume that $\Phi(0) < 0$, and the generalized Fourier transform $\widehat{\Phi}$ of Φ is continuous on $\mathbb{R}^d \setminus \{0\}$. Then the Pontryagin native space \mathcal{P} of K consists of all continuous functions of the form

$$\alpha\Phi + f, \quad \text{where } \alpha \in \mathbb{R}, \quad \widehat{f}/\sqrt{\widehat{\Phi}} \in L_2(\mathbb{R}^d),$$

and the indefinite inner product of \mathcal{P} is given by

$$(\alpha\Phi + f, \beta\Phi + g)_\mathcal{P} = \alpha\beta\Phi(0) + \beta f(0) + \alpha g(0) + \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{\widehat{f}(\omega)\overline{\widehat{g}(\omega)}}{\widehat{\Phi}(\omega)} d\omega.$$

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