

Multivariate Interpolation with Increasingly Flat Radial Basis Functions of Finite Smoothness

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Abstract

In this paper, we consider multivariate interpolation with radial basis functions of finite smoothness. In particular, we show that interpolants by radial basis functions in \mathbb{R}^d with finite smoothness of even order converge to a polyharmonic spline interpolant as the scale parameter of the radial basis functions goes to zero, i.e., the radial basis functions become increasingly flat.

1 Introduction

Radial basis functions (RBFs) have gained popularity over the last few decades in a variety of areas such as multivariate interpolation, approximation theory, meshless methods, neural networks, and machine learning. RBFs are typically used to approximate an unknown function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ in the following form

$$s(\mathbf{x}) = \sum_{j=1}^n \lambda_j \phi(\|\mathbf{x} - \mathbf{x}_j\|), \quad (1.1)$$

where $X := \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\} \subset \mathbb{R}^d$, are given scattered data sites, $\phi : [0, \infty) \rightarrow \mathbb{R}$ is a radial basic function, and $\|\cdot\|$ denotes the Euclidean distance. In what follows, we will assume the Fourier transform $\hat{\phi}$ of the RBF ϕ to be nonnegative on \mathbb{R}^d and positive at least on an open set of \mathbb{R}^d . In the case of multivariate interpolation, the expansion coefficients $\boldsymbol{\lambda} := (\lambda_1, \dots, \lambda_n)^T$ are obtained by solving the linear system

$$\mathbf{A}\boldsymbol{\lambda} = \mathbf{f}, \quad (1.2)$$

where $\mathbf{A} := [\phi(\|\mathbf{x}_j - \mathbf{x}_l\|)]_{j,l=1}^n$ and $\mathbf{f} := (f(\mathbf{x}_1), \dots, f(\mathbf{x}_n))^T$ represents the given data. By construction, the function obtained from (1.1) and (1.2) interpolates the function f at the scattered points $\mathbf{x}_1, \dots, \mathbf{x}_n$.

Many of the commonly used kernels contain a shape parameter in the following way

$$\phi_\epsilon(r) := \phi(\epsilon r), \quad \epsilon, r \geq 0. \quad (1.3)$$

If ϵ is very small, then the basic function ϕ_ϵ becomes increasingly flat. Moreover, with a very small ϵ , we have good approximation properties for both interpolation problems and solving elliptic partial differential equations (see [9, 6, 7, 14]). The condition of system (1.2) is, however, quite large for small ϵ (see [15]). A so-called “uncertainty relation” or “trade-off principle” quantifying these conflicting effects of having a small shape parameter have been analyzed in the literature (see, e.g., [12, 16]). However, it needs to be noted that the trade-off principle holds only if one follows the direct approach outlined above and uses the matrix \mathbf{A} to compute the expansion coefficients $\boldsymbol{\lambda}$. Alternative approaches that lead to stable and accurate numerical algorithms for very flat ϕ_ϵ are presented, e.g., in [6, 5]. However, we will not discuss these approaches in this paper. We concentrate on the limiting behavior of the interpolants

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as $\epsilon \rightarrow 0$. It was observed in [2] and later proved in [8, 9, 13] that, for infinitely smooth basic functions $\phi(\|\cdot\|)$, the limit as $\epsilon \rightarrow 0$ of the interpolant obtained from (1.1) and (1.2) is a multivariate polynomial provided some mild assumptions on ϕ and the data points X hold.

Previous work on flat RBFs has concentrated on infinitely smooth basic functions since they are known to yield spectral approximation orders. However, RBFs with finite smoothness are also of importance, especially in the setting of random fields. Often one has no *a priori* information of the smoothness of the interpolation problems in the random field setting. Therefore it was suggested in [17] that one should allow flexibility in the smoothness of the random field instead of assuming infinite smoothness. As a specific type of RBF with finite smoothness, Matérn kernels were investigated there.

We will focus on the discussion of the limit of multivariate interpolants using RBFs with finite smoothness. The motivation for this paper comes from our interest in the limiting behavior of interpolation with Matérn kernels. It was shown in [4] that many RBF kernels can be computed via a related Green's function with respect to an appropriate differential operator L . It turns out that the operator associated with the Matérn kernel “converges” to the operator associated with the polyharmonic splines as the shape parameter $\epsilon \rightarrow 0$ (see [4]). It is natural to ask whether the interpolants with Matérn functions also “converge” to the interpolants with polyharmonic splines as $\epsilon \rightarrow 0$. We will confirm this conjecture by showing that the interpolants based on a class of RBFs with finite smoothness converge to polyharmonic splines interpolants. As a consequence, we now know that a large class of infinitely smooth RBF interpolants converge to polynomial interpolants, and, similarly, a large class of RBF interpolants with finite smoothness converge to polyharmonic splines. Since univariate polynomial splines are commonly viewed as a piecewise smooth version of univariate polynomials we suggest that the new insight from this paper provides us with additional evidence that multivariate polyharmonic splines should (not only from a variational point of view) be considered as the natural generalization of univariate polynomial splines.

Specifically, we study in this paper RBFs of finite smoothness belonging to the following class. We consider any RBF ϕ with the following series expansion around 0:

$$\phi(r) = \sum_{k=0}^{\infty} c_k r^k, \quad (1.4)$$

where $c_{2v+1} \neq 0$ for some integer v and $c_{2k+1} = 0$ for $0 \leq k \leq v-1$. We denote this class of RBFs by $FS(v)$.

We point out that if the coefficients of all odd powers in (1.4) are zero, that is $v = \infty$, then $FS(v)$ reduces to the set of infinitely smooth RBFs. A typical example of an RBF with finite smoothness is the C^{2v} Matérn kernel (see [17, 3]):

$$\phi(r) = \frac{K_{v+\frac{d}{2}}(r)r^{v+\frac{d}{2}}}{2^{v-\frac{d}{2}}\Gamma(v+\frac{1}{2})}, \quad v \in \mathbb{N}_0,$$

where K_ν is the *modified Bessel function of the second kind* of order ν . Matérn kernels have also been referred to as Sobolev spline kernels [11] since they are known to be reproducing kernels of Sobolev spaces $H^{v+1}(\mathbb{R}^d)$ whenever $v+1 > \frac{d}{2}$. The C^{2v} Matérn kernel can be expanded in the form of (1.4) with $c_{2v+1} \neq 0$ and $c_{2k+1} = 0$ for $0 \leq k \leq v-1$ (see [17]). In [1, Ch. 6, Sect. 1.6] the authors discuss alternate reproducing kernels for the Sobolev space $H^{v+1}(\mathbb{R})$ corresponding to a different Hilbert space norm. We list some Matérn kernels and Sobolev kernels from [1] as examples in Table 1.

Since we consider the kernel with a shape parameter in the form of (1.3), we highlight the dependence of the interpolant in (1.1) on ϵ as

$$s(\mathbf{x}, \epsilon) := \sum_{j=1}^n \lambda_j(\epsilon) \phi_\epsilon(\|\mathbf{x} - \mathbf{x}_j\|), \quad (1.5)$$

$\phi(r) = e^{-r} = 1 - r + \frac{1}{2}r^2 - \frac{1}{6}r^3 + \dots$	C^0 Matérn ($d = 1$)
$\phi(r) = (1 + r)e^{-r} = 1 - \frac{1}{2}r^2 + \frac{1}{3}r^3 - \frac{1}{8}r^4 + \dots$	C^2 Matérn ($d = 1$)
$\phi(r) = (3 + 3r + r^2)e^{-r} = 3 - \frac{1}{2}r^2 + \frac{1}{8}r^4 - \frac{1}{15}r^5 + \frac{1}{48}r^6 + \dots$	C^4 Matérn ($d = 1$)
$\phi(r) = \frac{\sqrt{2}}{2}e^{-r} \sin\left(r + \frac{\pi}{4}\right) = \frac{1}{2} - \frac{1}{2}r^2 + \frac{1}{3}r^3 - \frac{1}{12}r^4 + \dots$	kernel of $H^2(\mathbb{R})$ [1, $\tau = \sqrt{2}$]
$\phi(r) = \frac{1}{6}e^{-r} + \frac{1}{3}e^{-\frac{r}{2}} \sin\left(\frac{\sqrt{3}}{2}r + \frac{\pi}{6}\right) = \frac{1}{3} - \frac{1}{12}r^2 + \frac{1}{72}r^4 - \frac{1}{240}r^5 + \dots$	kernel of $H^3(\mathbb{R})$ [1, $\tau = 1$]

Table 1: Matérn functions and kernels of Sobolev spaces for different orders of smoothness.

where the corresponding matrix and coefficients are

$$\mathbf{A}(\epsilon) = [\phi_\epsilon(\|\mathbf{x}_i - \mathbf{x}_j\|)]_{i,j=1}^n \quad \text{and} \quad \boldsymbol{\lambda}(\epsilon) = \mathbf{A}(\epsilon)^{-1} \mathbf{f} \quad (1.6)$$

We use $\pi_m(\mathbb{R}^d)$, $m \in \mathbb{N}$ to denote the set of polynomials in d variables of degree less than or equal to m and $N_{m,d}$ to denote the dimension of $\pi_m(\mathbb{R}^d)$. We say a set of distinct points $\{\mathbf{y}_j : j = 1, 2, \dots, N\} \subset \mathbb{R}^d$ is *unisolvant* with respect to $\pi_m(\mathbb{R}^d)$ if for any choice of $N_{m,d}$ linearly independent basis functions $\{p_l : l = 1, 2, \dots, N_{m,d}\}$ from $\pi_m(\mathbb{R}^d)$, there is a unique linear combination $\sum_{l=1}^{N_{m,d}} \beta_l p_l$ interpolating any given data over the set of points. We next present the main result of this paper.

Theorem 1 *If $\phi \in FS(v)$ and X contains a unisolvant set with respect to $\pi_{2v}(\mathbb{R}^d)$, then the limit of the interpolant $s(\mathbf{x}, \epsilon)$ as $\epsilon \rightarrow 0$ has the form of a polyharmonic spline interpolant. Specifically,*

$$\lim_{\epsilon \rightarrow 0} s(\mathbf{x}, \epsilon) = \sum_{j=1}^n \alpha_j \|\mathbf{x} - \mathbf{x}_j\|^{2v+1} + \sum_{l=1}^{N_{v,d}} \beta_l p_l(\mathbf{x}),$$

where $\{p_l : l = 1, \dots, N_{v,d}\}$ denotes a basis of $\pi_v(\mathbb{R}^d)$. Moreover, the coefficients can be determined by solving the following linear system:

$$\begin{pmatrix} \mathbf{G} & \mathbf{P} \\ \mathbf{P}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{0} \end{pmatrix}, \quad (1.7)$$

where $\mathbf{G} = [\|\mathbf{x}_i - \mathbf{x}_j\|^{2v+1}]_{i,j=1}^n$, $\mathbf{P} = [p_l(\mathbf{x}_j)]_{j,l=1}^{n, N_{v,d}}$ and \mathbf{f} is as in (1.2).

The main task in this paper is to prove the above theorem. The technique used in our proofs is similar to the method given in [8, 9]. More specifically, we will expand the interpolant $s(\mathbf{x}, \epsilon)$ in terms of powers of ϵ and establish the limit of $s(\mathbf{x}, \epsilon)$ exists by showing that the coefficients of negative powers of ϵ in the expansion are all zeros. Note that all the coefficients turn out to be polynomial functions of $\|\mathbf{x} - \mathbf{x}_j\|$. We divide the coefficients into two types: lower order polynomials of $\|\mathbf{x} - \mathbf{x}_j\|$ with degree no more than $2v$ and higher order polynomials of $\|\mathbf{x} - \mathbf{x}_j\|$ containing the term $\|\mathbf{x} - \mathbf{x}_j\|^{2v+1}$. Correspondingly, we arrange the proof in two steps. We first show that the coefficients in the form of lower order polynomials of $\|\mathbf{x} - \mathbf{x}_j\|$ with degree no more than $2v$ are zeros by using the assumptions $\phi \in FS(v)$ and the unisolvency of X . In order to prove that the coefficients in the form of higher order polynomials of $\|\mathbf{x} - \mathbf{x}_j\|$ containing the term $\|\mathbf{x} - \mathbf{x}_j\|^{2v+1}$ are zero we first obtain some moment conditions for these coefficients, and then use them together with the conditional positive definiteness of $\|\cdot\|^{2v+1}$ to obtain the desired result.

This paper is organized into 5 sections. In next section we expand $s(\mathbf{x}, \epsilon)$ in terms of powers of ϵ and show that the expansion coefficients are lower order polynomials of $\|\mathbf{x} - \mathbf{x}_j\|$ with degree no more than $2v$ which are zero. In Section 3, we present the moment conditions obtained from setting the coefficients in the form of lower order polynomials to be zero. We finally give a complete proof of Theorem 1 in Section 4 by showing that the coefficients in the form of higher order polynomials of $\|\mathbf{x} - \mathbf{x}_j\|$ are also zero based on the moment conditions obtained in Section 3. The result concerning interpolation with Matérn kernels will be presented as an immediate corollary there. Some numerical experiments to illustrate our result are shown in Section 5.

2 Power series expansion of the interpolant $s(\mathbf{x}, \epsilon)$

In this section, we will rewrite the interpolant $s(\mathbf{x}, \epsilon)$ in terms of powers of ϵ and first show that the expansion coefficients are given in the form of polynomials of $\|\mathbf{x} - \mathbf{x}_j\|$. We then establish that those coefficients with degree no more than $2v$ are zero. To this end, we first introduce some notation used throughout this paper. We define $\mathbb{N}_0 := \{0, 1, 2, \dots\}$ and for any $\mathbf{j} := (j_1, j_2, \dots, j_d) \in \mathbb{N}_0^d$ we let

$$|\mathbf{j}| := \sum_{l=1}^d j_l, \quad \text{and} \quad \mathbf{j}! := j_1! j_2! \cdots j_d!.$$

For any $\mathbf{b} := (b_1, b_2, \dots, b_d) \in \mathbb{R}^d$, let

$$\mathbf{b}^{\mathbf{j}} := b_1^{j_1} b_2^{j_2} \cdots b_d^{j_d}, \quad \mathbf{j} \in \mathbb{N}_0^d \quad \text{and} \quad \mathbf{b}^t := (b_1^t, b_2^t, \dots, b_d^t), \quad t \in \mathbb{N}_0.$$

For any $\mathbf{x} \in X$, we define

$$\mathbf{g}(\mathbf{x}) := (\|\mathbf{x} - \mathbf{x}_1\|, \|\mathbf{x} - \mathbf{x}_2\|, \dots, \|\mathbf{x} - \mathbf{x}_n\|)^T.$$

We next give a specific form of $s(\mathbf{x}, \epsilon)$ in terms of the powers of ϵ . Suppose $\phi \in FS(v)$ and write ϕ_ϵ in terms of powers of ϵ

$$\phi_\epsilon(r) = \phi(\epsilon r) = \sum_{k=0}^{\infty} c_k \epsilon^k r^k.$$

Formally, the coefficients $\lambda(\epsilon)$ in (1.6) can be obtained by Cramer's rule. It follows that they must be rational functions of ϵ since the entries of $\mathbf{A}(\epsilon)$ can be written as power series of ϵ . More specifically, there exists a positive integer τ such that for each $1 \leq j \leq n$

$$\lambda_j(\epsilon) = \epsilon^{-\tau} \sum_{\ell=0}^{\infty} a_{j,\ell} \epsilon^\ell, \tag{2.1}$$

for some sequence of numbers $(a_{j,0}, a_{j,1}, \dots)$. We can assume $\tau \geq 2v + 1$ without loss of generality (otherwise we can make τ large enough by taking the coefficients $a_{j,\ell} = 0$ for some missing j 's). Substituting these two above equalities into (1.5), we obtain an expansion of $s(\mathbf{x}, \epsilon)$ in terms of powers of ϵ :

$$s(\mathbf{x}, \epsilon) = \sum_{t=0}^{\infty} \varphi_t(\mathbf{x}) \epsilon^{-\tau+t},$$

where

$$\varphi_t(\mathbf{x}) = \sum_{k=0}^t c_k \mathbf{a}_{t-k}^T \mathbf{g}^k(\mathbf{x}), \quad \mathbf{a}_k = (a_{1,k}, \dots, a_{n,k})^T, \quad k \in \mathbb{N}_0. \tag{2.2}$$

To show the limit of $s(\mathbf{x}, \epsilon)$ exists, we need to show that $\varphi_t(\mathbf{x}) \equiv 0$ for all $0 \leq t \leq \tau - 1$, i.e., the expansion contains no negative powers of ϵ . Since $s(\cdot, \epsilon)$ interpolates \mathbf{f} at X for any $\epsilon > 0$, φ_t interpolates 0 at X for any $t \neq \tau$ and φ_τ interpolates \mathbf{f} at X . The next result shows that $\varphi_t(\mathbf{x}) \equiv 0$ for any $0 \leq t \leq 2v$ if X contains a unisolvent set with respect to $\pi_{2v}(\mathbb{R}^d)$.

Lemma 2 *If $\phi \in FS(v)$ and X contains a unisolvent set with respect to $\pi_{2v}(\mathbb{R}^d)$, then*

$$\varphi_t(\mathbf{x}) \equiv 0 \quad \text{for } 0 \leq t \leq 2v.$$

Proof: Since $\phi \in FS(v)$, $c_{2k+1} = 0$ for $0 \leq k \leq v - 1$. It follows from (2.2) that for $0 \leq t \leq 2v < \tau$, φ_t is a radial polynomial and belongs to $\pi_{2v}(\mathbb{R}^d)$. If X contains a unisolvent set with respect to $\pi_{2v}(\mathbb{R}^d)$, then $\varphi_t(\mathbf{x}) \equiv 0$ for any $0 \leq t \leq 2v$ since φ_t interpolates 0 at X for any $0 \leq t \leq 2v$. \square

We will show $\varphi_t \equiv 0$ for $2v + 1 \leq t \leq \tau - 1$ in the next two sections.

3 Discrete moment conditions

To show $\varphi_t \equiv 0$ for $2v + 1 \leq t \leq \tau - 1$, we need to use certain discrete moment conditions of \mathbf{a}_j and the conditional positive definiteness of the function $\mathbf{x} \mapsto \|\mathbf{x}\|^{2v+1}$. We present in this section the discrete moment conditions of \mathbf{a}_k obtained from $\varphi_t(\mathbf{x}) \equiv 0$, $0 \leq t \leq 2v$. To this end, we first review the definition of discrete moment conditions. Let I_t , where $t \in \mathbb{N}_0$, be the lexicographically ordered sequence of all multi-indices $\mathbf{k} \in \mathbb{N}_0^d$ such that $|\mathbf{k}| = t$ and $I_{\leq t}$ be the ordered sequence of all multi-indices $\mathbf{k} \in \mathbb{N}_0^d$ such that $|\mathbf{k}| \leq t$. The *discrete moment* of $\mathbf{b} \in \mathbb{R}^n$ with respect to X is defined as

$$\boldsymbol{\mu}_t(\mathbf{b}) := (\mu_{\mathbf{k}}(\mathbf{b}) : \mathbf{k} \in I_t)^T \quad \text{for } t \in \mathbb{N}_0, \quad (3.1)$$

where

$$\mu_{\mathbf{k}}(\mathbf{b}) := \sum_{j=1}^n b_j \mathbf{x}_j^{\mathbf{k}}, \quad \mathbf{k} \in \mathbb{N}_0^d. \quad (3.2)$$

The set of vectors satisfying *discrete moment conditions of order* $m \in \mathbb{N}$ with respect to X is

$$MC_m := \{\mathbf{b} \in \mathbb{R}^n : \boldsymbol{\mu}_t(\mathbf{b}) = 0 \text{ for any } 0 \leq t < m\}.$$

To be consistent with our notation, we let

$$MC_m := \mathbb{R}^n \quad \text{for } m \leq 0.$$

We will next present the discrete moment conditions of the coefficients \mathbf{a}_k in (2.2). To this end, we define a general form of radial polynomials for φ_t when $0 \leq t \leq 2v$. For any $t \in \mathbb{N}_0$ and $\{\mathbf{b}_0, \mathbf{b}_1, \dots, \mathbf{b}_t\} \subset \mathbb{R}^n$, let

$$p_t(\mathbf{x}, \mathbf{b}_0, \dots, \mathbf{b}_t) := \sum_{k=0}^{\lfloor \frac{t}{2} \rfloor} c_{2k} \mathbf{b}_{t-2k}^T \mathbf{g}^{2k}(\mathbf{x}), \quad (3.3)$$

where $c_k := \frac{\phi^{(k)}(0)}{k!}$, $k \in \mathbb{N}_0$. We can immediately observe that $p_t(\mathbf{x}, \mathbf{a}_0, \dots, \mathbf{a}_t) = \varphi_t(\mathbf{x})$ for $0 \leq t \leq 2v$. We define a few more quantities that we need in our proof. For any $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}_0^d$ and $|\boldsymbol{\alpha} + \boldsymbol{\beta}| = 2m$ with $m \in \mathbb{N}_0$, let

$$B(\boldsymbol{\alpha}, \boldsymbol{\beta}) := c_{2m} (-1)^{|\boldsymbol{\alpha}|} \frac{m!}{\left(\frac{\boldsymbol{\alpha} + \boldsymbol{\beta}}{2}\right)!} \frac{(\boldsymbol{\alpha} + \boldsymbol{\beta})!}{\boldsymbol{\alpha}! \boldsymbol{\beta}!}. \quad (3.4)$$

For any $k, l \in \mathbb{N}_0$, let

$$\mathbf{E}_{k,l} := [B(\boldsymbol{\alpha}, \boldsymbol{\beta})]_{\boldsymbol{\alpha} \in I_{2k}, \boldsymbol{\beta} \in I_{2l}} \quad \text{and} \quad \mathbf{W}_{k,l} := [B(\boldsymbol{\alpha}, \boldsymbol{\beta})]_{\boldsymbol{\alpha} \in I_{2k+1}, \boldsymbol{\beta} \in I_{2l+1}}. \quad (3.5)$$

We define two matrices for any $m \in \mathbb{N}_0$

$$\mathbf{E}_m := [\mathbf{E}_{k,l}]_{k,l=0}^m \quad \text{and} \quad \mathbf{W}_m := [\mathbf{W}_{k,l}]_{k,l=0}^m. \quad (3.6)$$

It was proved in [9] that both \mathbf{E}_m and \mathbf{W}_m are nonsingular for any $m \in \mathbb{N}_0$ if the Fourier transform $\hat{\phi}$ of the RBF ϕ is nonnegative on \mathbb{R}^d and positive at least on an open set of \mathbb{R}^d .

We have the following result on the discrete moment conditions of the coefficients of radial polynomials p_t that are zero functions.

Lemma 3 *Suppose $N \in \mathbb{N}_0$ and $\{\mathbf{b}_0, \mathbf{b}_1, \dots, \mathbf{b}_N\} \subset \mathbb{R}^n$. If $p_t(\mathbf{x}, \mathbf{b}_0, \dots, \mathbf{b}_t) \equiv 0$ for any $0 \leq t \leq N$, then*

$$\mathbf{b}_{2k} \in MC_{\lfloor \frac{N+2}{2} - 2k \rfloor}, \quad \mathbf{b}_{2k+1} \in MC_{\lfloor \frac{N+1}{2} - 2k \rfloor}, \quad \text{for } 0 \leq k \leq \left\lfloor \frac{N+1}{4} \right\rfloor. \quad (3.7)$$

Proof: We need to use the fact that both \mathbf{E}_m and \mathbf{W}_m are nonsingular for any $m \in \mathbb{N}_0$ (see [9]).

We will prove the desired result by induction. We first show the result holds for $N = 0$. In this case we only need to show that $\mathbf{b}_0 \in MC_1$. It follows from $p_0(\mathbf{x}, \mathbf{b}_0) = 0$ and (3.3) that

$$c_0 \mathbf{b}_0^T \mathbf{1} = 0, \quad \text{where } \mathbf{1} := (1, \dots, 1)^T.$$

Since $c_0 = \mathbf{E}_0$, it follows from the non-singularity of \mathbf{E}_0 that $c_0 \neq 0$. We have $\mathbf{b}_0^T \mathbf{1} = 0$, i.e., $\mathbf{b}_0 \in MC_1$.

Suppose the desired result holds for $N = 4\ell$ for some $\ell \in \mathbb{N}_0$. We prove that it also holds for $N = 4\ell + 1, 4\ell + 2, 4\ell + 3, 4\ell + 4$. We begin with the discussion of $N = 4\ell + 1$, i.e., we will show that

$$\mathbf{b}_{2k} \in MC_{2\ell+1-2k}, \quad \mathbf{b}_{2k+1} \in MC_{2\ell+1-2k}, \quad 0 \leq k \leq \ell.$$

Since (3.7) holds for $N = 4\ell$ by assumption, we have that

$$\mathbf{b}_{2k} \in MC_{2\ell+1-2k}, \quad \mathbf{b}_{2k+1} \in MC_{2\ell-2k}, \quad 0 \leq k \leq \ell,$$

and we only need to show

$$\boldsymbol{\mu}_{2\ell-2k}(\mathbf{b}_{2k+1}) = 0, \quad 0 \leq k \leq \ell. \quad (3.8)$$

We will prove this by using the fact that the coefficients of all powers of \mathbf{x} in p_t are zeros if $p_t \equiv 0$. For any $0 \leq l \leq \ell$ and $\boldsymbol{\alpha} \in I_{2l}$, let $p|_{\mathbf{x}^\alpha}$ be the coefficient of \mathbf{x}^α in $p_{2\ell+2l+1}(\mathbf{x}, \mathbf{b}_0, \dots, \mathbf{b}_{2\ell+2l+1})$. A direct calculation from (3.3) yields that

$$p|_{\mathbf{x}^\alpha} = \sum_{k=l}^{\ell+1} c_{2k} \mathbf{b}_{2\ell+2l+1-2k}^T \sum_{\boldsymbol{\beta} \in I_{2k-2l}} (-1)^{|\boldsymbol{\alpha}|} \frac{k!}{\left(\frac{\boldsymbol{\alpha}+\boldsymbol{\beta}}{2}\right)!} \frac{(\boldsymbol{\alpha}+\boldsymbol{\beta})!}{\boldsymbol{\alpha}! \boldsymbol{\beta}!} (\mathbf{x}_1^\beta, \dots, \mathbf{x}_n^\beta)^T.$$

This combined with the definition of $\boldsymbol{\mu}_k(\mathbf{a})$ in (3.2) and the definition of $B(\boldsymbol{\alpha}, \boldsymbol{\beta})$ in (3.4) yields that

$$p|_{\mathbf{x}^\alpha} = \sum_{k=l}^{\ell+1} \sum_{\boldsymbol{\beta} \in I_{2k-2l}} B(\boldsymbol{\alpha}, \boldsymbol{\beta}) \boldsymbol{\mu}_\beta(\mathbf{b}_{2\ell+2l+1-2k}).$$

Let $k := k + l$ in the right-hand side of the above equality. Then we have

$$p|_{\mathbf{x}^\alpha} = \sum_{k=0}^{\ell} \sum_{\boldsymbol{\beta} \in I_{2k}} B(\boldsymbol{\alpha}, \boldsymbol{\beta}) \boldsymbol{\mu}_\beta(\mathbf{b}_{2\ell+1-2k}).$$

Let $p|_{\mathbf{x}^{2l}} := (p|_{\mathbf{x}^\alpha} : \alpha \in I_{2l})^T$. It follows from the above equality, the definition of $\mathbf{E}_{k,l}$ in (3.5) and the definition of $\boldsymbol{\mu}_t(\mathbf{b})$ in (3.1) that

$$p|_{\mathbf{x}^{2l}} = \sum_{k=0}^{\ell} \mathbf{E}_{l,k} \boldsymbol{\mu}_{2k}(\mathbf{b}_{2\ell+1-2k}).$$

If $p_t(\mathbf{x}, \mathbf{b}_0, \dots, \mathbf{b}_t) = 0$ for any $\mathbf{x} \in \mathbb{R}^d$ and $0 \leq t \leq 4\ell + 1$, then $p|_{\mathbf{x}^{2l}} = 0$ for all $0 \leq l \leq \ell$. That is,

$$\mathbf{E}_\ell \cdot (\boldsymbol{\mu}_{2k}(\mathbf{b}_{2\ell+1-2k}) : k = 0, \dots, \ell)^T = 0.$$

Since \mathbf{E}_ℓ is nonsingular, we have that

$$\boldsymbol{\mu}_{2k}(\mathbf{b}_{2\ell+1-2k}) = 0, \quad 0 \leq k \leq \ell,$$

which implies (3.8).

We next show that the desired result holds with $N = 4\ell + 2$. One can easily see that it is enough to show

$$\boldsymbol{\mu}_{2\ell+1-2k}(\mathbf{b}_{2k}) = 0, \quad 0 \leq k \leq \ell. \quad (3.9)$$

Similar to the proof for the case $N = 4\ell + 1$, we can obtain the following linear system by setting the coefficients of \mathbf{x}^α in $p_{2\ell+2l+2}(\mathbf{x}, \mathbf{b}_0, \dots, \mathbf{b}_{2\ell+2l+2})$ for any $0 \leq l \leq \ell$ and $\alpha \in I_{2l+1}$ to zero

$$\mathbf{W}_\ell \cdot (\boldsymbol{\mu}_{2k+1}(\mathbf{b}_{2\ell-2k}) : k = 0, \dots, \ell)^T = 0.$$

Then (3.9) follows from the non-singularity of \mathbf{W}_ℓ .

We proceed with the proof for $N = 4\ell + 3$. That is, we need to show

$$\boldsymbol{\mu}_{2\ell+1-2k}(\mathbf{b}_{2k+1}) = 0, \quad 0 \leq k \leq \ell. \quad (3.10)$$

We obtain the following linear system by setting the coefficients of \mathbf{x}^α in $p_{2\ell+2l+3}(\mathbf{x}, \mathbf{b}_0, \dots, \mathbf{b}_{2\ell+2l+3})$ for any $0 \leq l \leq \ell$ and $\alpha \in I_{2l+1}$ to zero

$$\mathbf{W}_\ell \cdot (\boldsymbol{\mu}_{2k+1}(\mathbf{b}_{2\ell+1-2k}) : k = 0, \dots, \ell)^T = 0.$$

Then (3.10) follows from the non-singularity of \mathbf{W}_ℓ .

It remains to prove the desired result holds for $N = 4\ell + 4$. We need to show that

$$\boldsymbol{\mu}_{2\ell+2-2k}(\mathbf{b}_{2k}) = 0, \quad 0 \leq k \leq \ell + 1. \quad (3.11)$$

Setting the coefficients of \mathbf{x}^α in $p_{2\ell+2l+2}(\mathbf{x}, \mathbf{b}_0, \dots, \mathbf{b}_{2\ell+2l+2})$ for any $0 \leq l \leq \ell + 1$ and $\alpha \in I_{2l}$ to zero, we have that

$$\mathbf{E}_{\ell+1} \cdot (\boldsymbol{\mu}_{2k}(\mathbf{b}_{2\ell+2-2k}) : k = 0, \dots, \ell + 1)^T = 0.$$

Then (3.11) follows from the non-singularity of $\mathbf{E}_{\ell+1}$. □

We are now ready to present the discrete moment conditions for the coefficients \mathbf{a}_k in (2.2).

Lemma 4 *If $\phi \in FS(v)$ and X contains a unisolvent set with respect to $\pi_{2v}(\mathbb{R}^d)$, then*

$$\mathbf{a}_{2k} \in MC_{v+1-2k}, \quad \mathbf{a}_{2k+1} \in MC_{v-2k}, \quad 0 \leq k \leq \left\lfloor \frac{v}{2} \right\rfloor.$$

Proof: One can immediately observe that if $\phi \in FS(v)$, then

$$\phi_t(\mathbf{x}) = p_t(\mathbf{x}, \mathbf{a}_0, \dots, \mathbf{a}_t), \quad 0 \leq t \leq 2v.$$

It follows from Lemma 2 that

$$p_t(\mathbf{x}, \mathbf{a}_0, \dots, \mathbf{a}_t) \equiv 0, \quad 0 \leq t \leq 2v.$$

The desired result follows from this combined with Lemma 3. □

4 The limit of the interpolant: a proof of Theorem 1

To prove Theorem 1, we need to show $\varphi_t \equiv 0$ for $0 \leq t \leq \tau - 1$. We already proved in Lemma 1 that $\varphi_t \equiv 0$ for $0 \leq t \leq 2v$. It suffices to show that $\tau = 2v + 1$. For this purpose, we first review the definition of *conditional positive definiteness* that will be used in the proof. We call a continuous function $\psi : \mathbb{R}^d \rightarrow \mathbb{R}$ *conditionally positive definite of order m* if for all $N \in \mathbb{N}$, every finite set of pairwise distinct centers $Y := \{\mathbf{y}_1, \dots, \mathbf{y}_N\} \subset \mathbb{R}^d$, and every $\boldsymbol{\alpha} \in \mathbb{R}^N \setminus \{0\}$ satisfying

$$\sum_{j=1}^N \alpha_j p(\mathbf{y}_j) = 0, \quad p \in \pi_{m-1}(\mathbb{R}^d),$$

the quadratic form

$$\sum_{i,j=1}^N \alpha_i \alpha_j \psi(\mathbf{y}_i - \mathbf{y}_j)$$

is positive. Moreover, if ψ is conditionally positive definite of order m and X is unisolvent with respect to $\pi_{m-1}(\mathbb{R}^d)$, then we have a unique interpolant to a function f at X in the following form

$$\sum_{j=1}^N \alpha_j \psi(\mathbf{x} - \mathbf{y}_j) + \sum_{l=1}^{N_{m-1,d}} \beta_l p_l(\mathbf{x})$$

with the additional conditions

$$\sum_{j=1}^N \alpha_j p_l(\mathbf{y}_j) = 0, \quad 1 \leq l \leq N_{m-1,d},$$

where $\{p_l : 1 \leq l \leq N_{m-1,d}\}$ is a basis of $\pi_{m-1,d}$. That is, the following system

$$\begin{pmatrix} \mathbf{A}_{\psi,Y} & \mathbf{P} \\ \mathbf{P}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix} = \begin{pmatrix} \mathbf{f}|_Y \\ \mathbf{0} \end{pmatrix}, \quad (4.1)$$

where $\mathbf{A}_{\psi,Y} = [\psi(\mathbf{y}_i - \mathbf{y}_j)]_{i,j=1}^N$, $\mathbf{P} = [p_l(\mathbf{y}_j)]_{j,l=1}^{N,N_{m-1,d}}$ and $\mathbf{f}|_Y = (f(\mathbf{y}_j) : j = 1, \dots, N)^T$, is uniquely solvable.

The next result gives an explicit form of $\varphi_{2v+1}(\mathbf{x})$.

Lemma 5 *If $\phi \in FS(v)$ and X contains a unisolvent set with respect to $\pi_{2v}(\mathbb{R}^d)$, then*

$$\varphi_{2v+1}(\mathbf{x}) = c_0 \mathbf{a}_0^T \mathbf{g}^{2v+1}(\mathbf{x}) + q(\mathbf{x}),$$

for some $q(\mathbf{x}) \in \pi_v(\mathbb{R}^d)$.

Proof: Since $\phi \in FS(v)$, $c_{2k+1} = 0$ for $0 \leq k \leq v - 1$. It follows from (2.2) that

$$\varphi_{2v+1}(\mathbf{x}) = c_0 \mathbf{a}_0^T \mathbf{g}^{2v+1}(\mathbf{x}) + \sum_{k=1}^v c_{2k} \mathbf{a}_{2v+1-2k}^T \mathbf{g}^{2k}(\mathbf{x}).$$

Let $q(\mathbf{x}) := \sum_{k=1}^v c_{2k} \mathbf{a}_{2v+1-2k}^T \mathbf{g}^{2k}(\mathbf{x})$. It remains to prove $q(\mathbf{x}) \in \pi_v(\mathbb{R}^d)$. That is, we need to show that the coefficient of \mathbf{x}^α in $q(\mathbf{x})$ is 0 if $|\alpha| \geq v + 1$. It follows from a direct calculation that for any α , the coefficient of \mathbf{x}^α in $q(\mathbf{x})$ is

$$q|_{\mathbf{x}^\alpha} = \sum_{k=\lfloor \frac{|\alpha|}{2} \rfloor}^v c_{2k} \mathbf{a}_{2v+1-2k}^T \sum_{\boldsymbol{\beta} \in I_{2k-|\alpha|}} (-1)^{|\alpha|} \frac{k!}{\left(\frac{\alpha+\boldsymbol{\beta}}{2}\right)!} \frac{(\alpha+\boldsymbol{\beta})!}{\alpha! \boldsymbol{\beta}!} (\mathbf{x}_1^\beta, \dots, \mathbf{x}_n^\beta)^T.$$

This combined with the definition of $\mu_k(\mathbf{a})$ in (3.2) and the definition of $B(\boldsymbol{\alpha}, \boldsymbol{\beta})$ in (3.4) yields that

$$q_{|\mathbf{x}^\alpha} = \sum_{k=\lfloor \frac{|\alpha|}{2} \rfloor}^v \sum_{\boldsymbol{\beta} \in I_{2k-|\alpha|}} B(\boldsymbol{\alpha}, \boldsymbol{\beta}) \mu_{\boldsymbol{\beta}}(\mathbf{a}_{2v+1-2k}).$$

It suffices to show that

$$\mu_{2k-|\alpha|}(\mathbf{a}_{2v+1-2k}) = 0, \quad \text{for } \left\lfloor \frac{|\alpha|}{2} \right\rfloor \leq k \leq v \text{ and } |\alpha| \geq v+1.$$

We will use the discrete moment conditions of the coefficients \mathbf{a}_k . It follows from Lemma 4 that for any $\left\lfloor \frac{|\alpha|}{2} \right\rfloor \leq k \leq v$ and $|\alpha| \geq v+1$

$$\mathbf{a}_{2v+1-2k} \in MC_{2k-v} \subset MC_{2k-|\alpha|+1},$$

which implies $\mu_{2k-|\alpha|}(\mathbf{a}_{2v+1-2k}) = 0$. \square

We are now ready to present the proof of Theorem 1 on the limit of $s(\mathbf{x}, \epsilon)$ as $\epsilon \rightarrow 0$.

Proof of Theorem 1: To show the existence of the limit of $s(\mathbf{x}, \epsilon)$ as $\epsilon \rightarrow 0$, it suffices to prove that we can take $\tau = 2v + 1$. Then it follows from Lemma 1 that $\varphi_t \equiv 0$ for $0 \leq t \leq \tau - 1$ which implies the limit of $s(\mathbf{x}, \epsilon)$ as $\epsilon \rightarrow 0$ exists.

Recall that φ_t interpolates 0 at X if $t \neq \tau$. If $\tau > 2v + 1$, then φ_{2v+1} also interpolates 0 at X . Since X contains a unisolvent set with respect to $\pi_{2v}(\mathbb{R}^d)$, it follows from Lemma 5 and the fact that $\mathbf{x} \mapsto \|\mathbf{x}\|^{2v+1}$ is conditionally positive definite of order $v + 1$ ([10, 18]) that $\varphi_{2v+1}(\mathbf{x}) \equiv 0$. Moreover,

$$\mathbf{a}_0 = 0.$$

This implies that the term $\epsilon^{-\tau}$ is not present in the expansion (2.1) of $\boldsymbol{\lambda}(\epsilon)$, i.e., we can let $\tau := \tau - 1$ and repeat the same process to conclude that there is no term of the form ϵ^{-k} in $\boldsymbol{\lambda}(\epsilon)$ whenever $k > 2v + 1$. Consequently, we can take $\tau = 2v + 1$ and the limit of $s(\mathbf{x}, \epsilon)$ is $\varphi_{2v+1}(\mathbf{x})$ as $\epsilon \rightarrow 0$. The desired result follows from Lemma 5 and the conditional positive definiteness of φ_{2v+1} . \square

The result for interpolation with Matérn kernels follows immediately.

Corollary 6 *If ϕ is the C^{2v} Matérn kernel, then $\phi \in FS(v)$. Moreover, if X contains a unisolvent set with respect to $\pi_{2v}(\mathbb{R}^d)$, then*

$$\lim_{\epsilon \rightarrow 0} s(\mathbf{x}, \epsilon) = \sum_{j=1}^n \alpha_j \|\mathbf{x} - \mathbf{x}_j\|^{2v+1} + \sum_{l=1}^{N_{v,d}} \beta_l p_l(\mathbf{x}),$$

where the coefficients α_j, β_l are uniquely determined by solving the linear system (1.7).

Proof: It was pointed out in [17] that the C^{2v} Matérn kernel can be expanded in the form of (1.4) with $c_{2v+1} \neq 0$ and $c_{2k+1} = 0$ for $0 \leq k \leq v - 1$. That is, the C^{2v} Matérn kernel belongs to $FS(v)$. The second result follows immediately from Theorem 1. \square

5 Numerical Experiments

In this section we present three numerical examples to illustrate the convergence behavior of interpolation with C^0 and C^2 Matérn kernels as well as a Sobolev kernel for $H^2(\mathbb{R})$ from [1] (see Table 1). For each example, we interpolate the values (0, 0.8, 1.5, 0.9, 1.1, 1.4) at (0, 0.5, 1.5, 3.5, 4, 5).

In the first example, we consider interpolation with the C^0 Matérn kernel $\phi_\epsilon(x) = e^{-\epsilon x}$ and the shape parameter ϵ takes the values 2, 1, and 0.1. The interpolants are shown in Figure 1.

In the second example, we consider interpolation with the C^2 Matérn kernel $\phi_\epsilon(x) = (1 + \epsilon x)e^{-\epsilon x}$ with values of the shape parameter ϵ ranging from 2, 1, to 0.1. The interpolants are shown in Figure 2.

For the third example we consider interpolation with the H^2 Sobolev kernel $\phi_\epsilon(x) = \frac{\sqrt{2}}{2}e^{-\epsilon x} \sin(\epsilon x + \frac{\pi}{4})$ with values of the shape parameter ϵ ranging from 2, 1, to 0.1. The interpolants are shown in Figure 3.

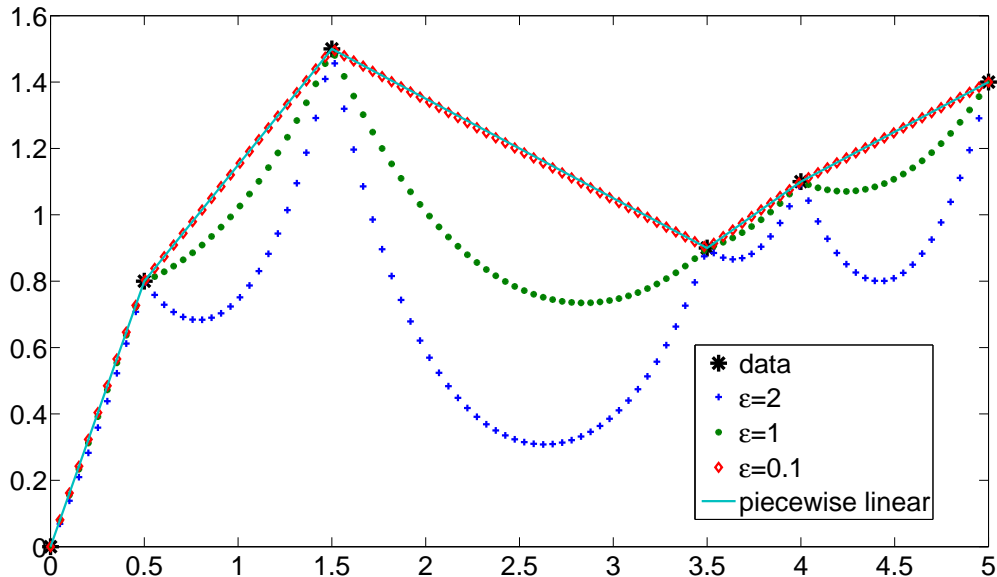


Figure 1: Convergence of C^0 Matérn interpolant to piecewise linear spline.

From all three examples presented here we can see that the interpolants with both types of finitely smooth kernels converge to the polyharmonic interpolants as the shape parameter ϵ goes to 0.

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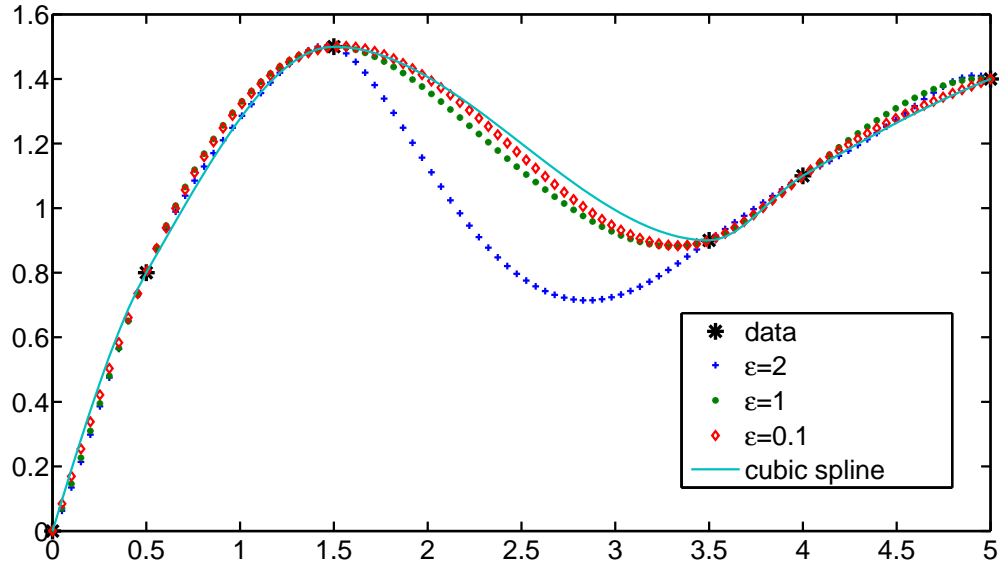


Figure 2: Convergence of C^2 Matérn interpolant to cubic spline.

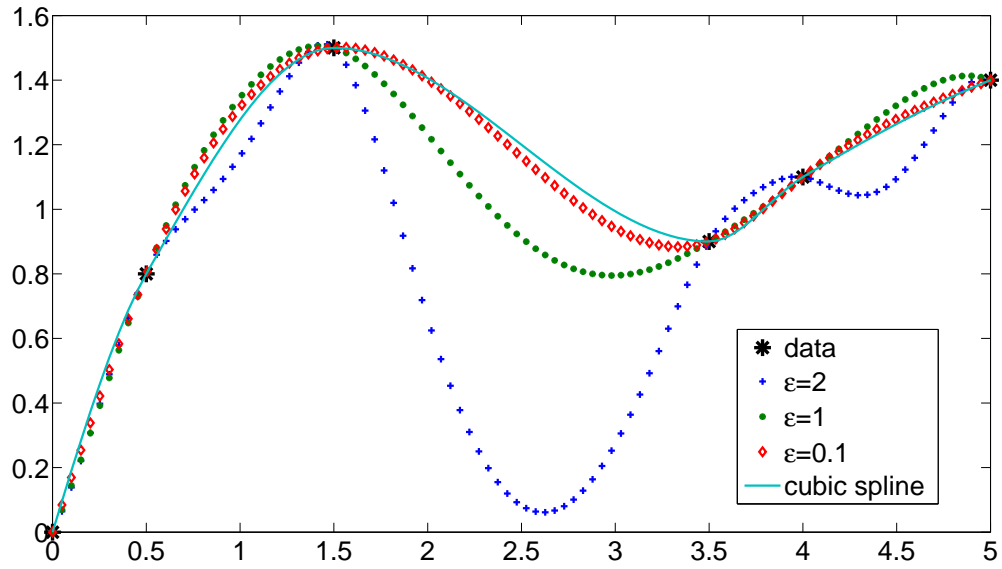


Figure 3: Convergence of H^2 kernel interpolant to cubic spline.

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