

On the Approximation Order and Numerical Stability of Local Lagrange Interpolation by Polyharmonic Splines

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Abstract

This paper proves convergence rates for local scattered data interpolation by polyharmonic splines. To this end, it is shown that the Lagrange basis functions of polyharmonic spline interpolation are invariant under uniform scalings. Consequences of this important result for the numerical stability of the local interpolation scheme are discussed. A stable algorithm for the evaluation of polyharmonic spline interpolants is proposed.

1 Introduction

Polyharmonic splines, also often referred to as *surface splines*, are powerful tools for multivariate scattered data interpolation (see [5, 10, 11] for surveys). In this problem, a data vector $f|_X = (f(x_1), \dots, f(x_n))^T \in \mathbb{R}^n$ of function values, sampled from an unknown function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ at a *scattered* point set $X = \{x_1, \dots, x_n\} \subset \mathbb{R}^d$, $d \geq 1$, is assumed to be given. Scattered data interpolation requires computing a *suitable* interpolant $s : \mathbb{R}^d \rightarrow \mathbb{R}$ satisfying $s|_X = f|_X$, i.e.,

$$s(x_j) = f(x_j), \quad \text{for all } 1 \leq j \leq n. \quad (1.1)$$

To this end, the polyharmonic spline interpolation scheme works with a fixed *radial* function,

$$\phi_{d,k}(r) = \begin{cases} r^{2k-d} \log(r), & \text{for } d \text{ even,} \\ r^{2k-d}, & \text{for } d \text{ odd,} \end{cases}$$

where $2k > d$, and with $k \in \mathbb{N}$. The interpolant s in (1.1) is required to have the form

$$s(x) = \sum_{j=1}^n c_j \phi_{d,k}(\|x - x_j\|) + p(x), \quad p \in \mathcal{P}_m^d, \quad (1.2)$$

where $\|\cdot\|$ is the Euclidean norm on \mathbb{R}^d . Moreover, \mathcal{P}_m^d denotes the linear space containing all real-valued polynomials in d variables of degree at most $m - 1$, where we let $m = k - \lceil d/2 \rceil + 1$ for the *order* of the conditionally positive (negative) definite function $\phi_{d,k}$. For more details concerning conditionally positive definite functions, see [19, 24].

By the n linear equations in the interpolation conditions (1.1), and by additionally requiring the q *vanishing moment conditions*

$$\sum_{j=1}^n c_j p(x_j) = 0, \quad \text{for all } p \in \mathcal{P}_m^d,$$

with $q = \binom{m-1+d}{d}$ being the dimension of \mathcal{P}_m^d , the $n + q$ unknown coefficients of s in (1.2) can be computed by solving the resulting linear system of size $(n + q) \times (n + q)$. This linear system has always a solution, which is unique, provided that the point set X is \mathcal{P}_m^d -*unisolvent* [19]. The latter is equivalent to requiring that there is no nontrivial polynomial in \mathcal{P}_m^d that vanishes on all points in X , i.e., for $p \in \mathcal{P}_m^d$ we have the implication

$$p(x_j) = 0 \quad \text{for } 1 \leq j \leq n \quad \implies \quad p \equiv 0.$$

Much of the ground-breaking work on the theory of polyharmonic spline interpolation was done by Duchon [7, 8, 9] and by Meinguet [17, 18] in the late 70s. Apart from fundamental questions concerning the solvability and uniqueness of polyharmonic spline interpolation, Duchon [7, 8, 9] did also address the central aspect of *convergence* and *convergence rates*, albeit for special cases, such as for *thin plate spline* interpolation in the plane, where $k = d = 2$, and therefore $\phi_{2,2} = r^2 \log(r)$. Since then, several improvements on various different aspects concerning the error analysis of scattered data interpolation by polyharmonic splines have been made [14, 15, 16, 21, 25, 26].

In the setting of these papers, the resulting convergence rates are, for a fixed bounded and open domain $\Omega \subset \mathbb{R}^d$ comprising X , $X \subset \Omega$, proven in terms of the *fill distance*

$$h_{X,\Omega} = \sup_{y \in \Omega} \min_{x \in X} \|y - x\|$$

of X in Ω . So were e.g. pointwise error estimates, due to Wu and Schaback [26], used in [25] in order to obtain, for functions f in the *native space* $\mathcal{F}_{\phi_{d,k}}$ of $\phi_{d,k}$, uniform error bounds of the form

$$\|f - s\|_{L_\infty(\Omega)} \leq C \cdot |f|_{\mathcal{F}_{\phi_{d,k}}} \cdot h_{X,\Omega}^{k-d/2}, \quad \text{for } f \in \mathcal{F}_{\phi_{d,k}}, \quad (1.3)$$

where Ω is required to satisfy an *interior cone condition*.

In this sense, the *approximation order* of polyharmonic spline interpolation is $p = k - d/2$ for functions f in the native function space $\mathcal{F}_{\phi_{d,k}}$. We remark that this approximation order can, due to Schaback [22], be doubled, but with requiring more regularity for f . Moreover, *saturation theorems* concerning special cases of polyharmonic spline interpolation are proven in [25].

This paper proves convergence rates for *local* Lagrange interpolation by polyharmonic splines. To this end, we consider for any fixed point x_0 and a \mathcal{P}_m^d -unisolvent point set $X = \{x_1, \dots, x_n\} \subset \mathbb{R}^d$ the interpolation problem

$$s^h(x_0 + hx_j) = f(x_0 + hx_j), \quad 1 \leq j \leq n, \quad (1.4)$$

in a local neighbourhood $U_h(x_0)$ of x_0 , where h is a positive scaling parameter. Due to our assumptions on X , there is for any $h > 0$ a unique polyharmonic spline interpolant s^h , using $\phi_{d,k}$, satisfying (1.4). The following Section 2 discusses further details concerning local polyharmonic spline interpolation.

Then, in Section 3 the convergence rate of polyharmonic spline interpolation is determined in terms of asymptotic bounds of the form

$$|s^h(x_0 + hx) - f(x_0 + hx)| = \mathcal{O}(h^p), \quad h \rightarrow 0, \quad (1.5)$$

in which case p is said to be the *approximation order* at x_0 . A precise definition of this term is given in Section 3, Definition 3.1. Note that this concept for a *local* convergence rate is in contrast to the *global* one above. Indeed, the bound in (1.3) is obtained for a small fill distance $h_{X,\Omega}$ of X in the fixed domain Ω . This requires a high density of X in the global domain Ω , whereas the asymptotic bound (1.5) is obtained by locally scaling the interpolation points relative to the center x_0 .

It is shown in Section 3 that the convergence rate p in (1.5) is, for functions f which are C^m locally around x_0 , given by the abovementioned order m of $\Phi_{d,k}$, i.e., $p = k - \lceil d/2 \rceil + 1$. Note that this is in contrast to the global case in (1.3), where we only obtain $p = k - d/2$ for functions in the native space $\mathcal{F}_{\phi_{d,k}}$.

In order to establish approximation orders for local interpolation, it is shown that the Lagrange basis functions of the polyharmonic spline interpolant s^h are invariant under scalings of h . This key observation, to be proven in Section 3, Lemma 3.2, is due to the homogeneity of the radial basis functions $\phi_{d,k}$. For a discussion on further consequences from this essential property of polyharmonic splines we refer to the related work [1].

The scale-invariance of the Lagrange basis allows us to draw further conclusions concerning the condition number of the interpolation problem (1.1) and the numerical stability of polyharmonic spline interpolation. These important aspects are subject of the discussion in Section 4, where a stable algorithm for evaluating the interpolant s^h is proposed for situations where the point set X is of *moderate* size, i.e., for *small* n .

We finally remark that the motivation for analyzing the approximation order and numerical stability of local polyharmonic spline interpolation comes from applications concerning the numerical simulation of multiscale phenomena in transport processes. To this end, an adaptive and meshfree method of backward characteristics for solving both linear and nonlinear transport equations is proposed in the previous papers [2, 4]. This particle-based Lagrangian advection scheme works with local Lagrange interpolation by polyharmonic splines, at a *small* number of scattered nodes, each of which corresponds (at a time t) to one flow particle. In this method, the local interpolation at the nodes is combined in order to obtain global approximations to the solution of a hyperbolic equation. The performance of this advection scheme essentially relies on both the approximation order and the numerical stability of local Lagrange interpolation. For further details on this, see [2, 3, 4].

2 Local Interpolation by Polyharmonic Splines

In this section, we recall selected basic features of polyharmonic spline interpolation, which are relevant for the following discussion in this text. Moreover, we introduce some notations. Starting point of the subsequent discussion is the *scaled* interpolation problem (1.4). Due to the shift-invariance of polyharmonic spline interpolation, we assume from now $x_0 = 0$ without loss of generality, so that (1.4) becomes

$$s^h(hx_j) = f(hx_j), \quad 1 \leq j \leq n. \quad (2.6)$$

For any $h > 0$, and a fixed \mathcal{P}_m^d -unisolvent point set X , the interpolation problem (2.6) has under constraints

$$\sum_{j=1}^n c_j^h p(hx_j) = 0, \quad \text{for all } p \in \mathcal{P}_m^d, \quad (2.7)$$

a unique solution s^h of the form

$$s^h(hx) = \sum_{j=1}^n c_j^h \phi_{d,k}(\|hx - hx_j\|) + \sum_{|\alpha| < m} d_\alpha^h (hx)^\alpha, \quad (2.8)$$

whose coefficients $c^h = (c_1^h, \dots, c_n^h)^T \in \mathbb{R}^n$ and $d^h = (d_\alpha^h)_{|\alpha| < m} \in \mathbb{R}^q$ can be computed by solving the linear system

$$\begin{bmatrix} \Phi_h & \Pi_h \\ \Pi_h^T & 0 \end{bmatrix} \cdot \begin{bmatrix} c^h \\ d^h \end{bmatrix} = \begin{bmatrix} f|_{hX} \\ 0 \end{bmatrix}, \quad (2.9)$$

where we let

$$\begin{aligned} \Phi_h &= (\phi_{d,k}(\|hx_i - hx_j\|))_{1 \leq i, j \leq n} \in \mathbb{R}^{n \times n}, \\ \Pi_h &= ((hx_i)^\alpha)_{1 \leq i \leq n; |\alpha| < m} \in \mathbb{R}^{n \times q}, \\ f|_{hX} &= (f(hx_i))_{1 \leq i \leq n} \in \mathbb{R}^n. \end{aligned}$$

In the following discussion it will be useful to abbreviate the above linear system (2.9) as

$$A_h \cdot b^h = f_h, \quad (2.10)$$

i.e., for the sake of notational brevity, we let

$$A_h = \begin{bmatrix} \Phi_h & \Pi_h \\ \Pi_h^T & 0 \end{bmatrix}, \quad b^h = \begin{bmatrix} c^h \\ d^h \end{bmatrix}, \quad \text{and} \quad f_h = \begin{bmatrix} f|_{hX} \\ 0 \end{bmatrix}.$$

We recall the *Lagrange representation* of s^h in (2.8), given by

$$s^h(hx) = \sum_{i=1}^n \lambda_i^h(hx) f(hx_i), \quad (2.11)$$

with the *Lagrange basis functions* λ_i^h satisfying

$$\lambda_i^h(hx_j) = \begin{cases} 1 & \text{for } i = j, \\ 0 & \text{for } i \neq j. \end{cases}$$

Moreover, due to the reproduction of polynomials from \mathcal{P}_m^d , we have

$$\sum_{i=1}^n \lambda_i^h(hx) p(hx_i) = p(hx), \quad \text{for all } p \in \mathcal{P}_m^d. \quad (2.12)$$

The Lagrange functions can pointwise, at any hx , be evaluated by solving the linear system

$$\begin{bmatrix} \Phi_h & \Pi_h \\ \Pi_h^T & 0 \end{bmatrix} \cdot \begin{bmatrix} \lambda^h(hx) \\ \mu^h(hx) \end{bmatrix} = \begin{bmatrix} \varphi_h(hx) \\ \pi_h(hx) \end{bmatrix}, \quad (2.13)$$

where we let $\lambda^h(hx) = (\lambda_i^h(hx))_{1 \leq i \leq n} \in \mathbb{R}^n$, and $\mu^h(hx) = (\mu_\alpha^h(hx))_{|\alpha| < m} \in \mathbb{R}^q$ for the vector of the *Lagrange multipliers*. Moreover, the right hand side

$$\begin{aligned} \varphi_h(hx) &= (\phi_{d,k}(\|hx - hx_j\|))_{1 \leq j \leq n} \in \mathbb{R}^n, \\ \pi_h(hx) &= ((hx)^\alpha)_{|\alpha| < m} \in \mathbb{R}^q, \end{aligned}$$

in (2.13) contains the point evaluations of the basis functions at hx . Again, it is convenient to abbreviate the above system (2.13) by

$$A_h \cdot \nu^h(hx) = \beta_h(hx),$$

where we let

$$\nu^h(hx) = \begin{bmatrix} \lambda^h(hx) \\ \mu^h(hx) \end{bmatrix} \quad \text{and} \quad \beta_h(hx) = \begin{bmatrix} \varphi_h(hx) \\ \pi_h(hx) \end{bmatrix}.$$

Starting with the Lagrange representation of s^h in (2.11), we obtain

$$\begin{aligned} s^h(hx) &= \langle \lambda^h(hx), f|_{hX} \rangle \\ &= \langle \nu^h(hx), f_h \rangle \\ &= \langle A_h^{-1} \cdot \beta_h(hx), f_h \rangle \\ &= \langle \beta_h(hx), A_h^{-1} \cdot f_h \rangle \\ &= \langle \beta_h(hx), b_h \rangle, \end{aligned} \quad (2.14)$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product of the Euclidean space \mathbb{R}^d . This in particular combines the two alternative representations for s^h in (2.11) and (2.8).

3 Approximation Order

The discussion in this section is dominated by the following definition.

Definition 3.1. *Let s^h denote the polyharmonic spline interpolant, using $\phi_{d,k}$, satisfying (2.6). We say that the **approximation order** of local polyharmonic spline interpolation with respect to the function space \mathcal{F} is p , iff for any $f \in \mathcal{F}$ the asymptotic bound*

$$|f(hx) - s^h(hx)| = \mathcal{O}(h^p), \quad h \rightarrow 0,$$

holds for any $x \in \mathbb{R}^d$, and any finite \mathcal{P}_m^d -unisolvent point set $X \subset \mathbb{R}^d$.

Recall from the discussion in the previous Section 2 that any interpolant s^h satisfying (2.6) has a unique Lagrange representation of the form (2.11). The following lemma concerning the scale-invariance of the Lagrange basis plays a key role in the following discussion of this paper.

Lemma 3.2. *The Lagrange basis functions of polyharmonic spline interpolation are invariant under uniform scalings, i.e., for any $h > 0$, we have*

$$\lambda^h(hx) = \lambda^1(x), \quad \text{for every } x \in \mathbb{R}^d.$$

Proof. For $h > 0$, let

$$\mathcal{S}_h = \left\{ \sum_{j=1}^n c_j \phi_{d,k}(\|\cdot - hx_j\|) + p : p \in \mathcal{P}_m^d, \sum_{j=1}^n c_j q(x_j) = 0 \text{ for all } q \in \mathcal{P}_m^d \right\}$$

denote the space of all possible polyharmonic spline interpolants of the form (2.8) satisfying (2.7). In what follows, we show that \mathcal{S}_h is a scaled version of \mathcal{S}_1 , so that $\mathcal{S}_h = \{\sigma_h(s) : s \in \mathcal{S}_1\}$, where the dilatation operator σ_h is given by $\sigma_h(s) = s(\cdot/h)$. This then implies that, due to the unicity of the interpolation in either space, \mathcal{S}_h or \mathcal{S}_1 , their Lagrange basis functions satisfy $\lambda^h = \sigma_h(\lambda^1)$, as stated above.

In order to show that $\mathcal{S}_h = \sigma_h(\mathcal{S}_1)$, we distinguish the special case where d is even from the one where d is odd. If the space dimension d is odd, then $\mathcal{S}_h = \sigma_h(\mathcal{S}_1)$ follows immediately from the homogeneity of $\phi_{d,k}$, where $\phi_{d,k}(hr) = h^{2k-d} \phi_{d,k}(r)$.

Now suppose that d is even. In this case we have

$$\phi_{d,k}(hr) = h^{2k-d} \left(\phi_{d,k}(r) + r^{2k-d} \log(h) \right).$$

Therefore, any function $s^h \in \mathcal{S}_h$ has, for some $p \in \mathcal{P}_m^d$, the form

$$s^h(hx) = h^{2k-d} \left(\sum_{j=1}^n c_j \phi_{d,k}(\|x - x_j\|) + \log(h)r(x) \right) + p(x),$$

where we let

$$r(x) = \sum_{j=1}^n c_j \|x - x_j\|^{2k-d}.$$

In order to see that s^h is contained in $\sigma_h(\mathcal{S}_1)$, it remains to show that the degree of the polynomial r is at most $m - 1$. To this end, we rewrite r as

$$r(x) = \sum_{j=1}^n c_j \sum_{|\alpha|+|\beta|=2k-d} c_{\alpha,\beta} \cdot x^\alpha (x_j)^\beta = \sum_{|\alpha|+|\beta|=2k-d} c_{\alpha,\beta} \cdot x^\alpha \sum_{j=1}^n c_j (x_j)^\beta,$$

for some coefficients $c_{\alpha,\beta} \in \mathbb{R}$ with $|\alpha| + |\beta| = 2k - d$. Due to the vanishing moment conditions (2.7) for the coefficients c_1, \dots, c_n , this implies that the degree of r is at most $2k - d - m = k - d/2 - 1 < m$. Therefore, $s^h \in \sigma_h(\mathcal{S}_1)$, and so $\mathcal{S}_h \subset \sigma_h(\mathcal{S}_1)$. The inclusion $\mathcal{S}_1 \subset \sigma_h^{-1}(\mathcal{S}_h)$ can be proven accordingly.

Altogether, we find that $\mathcal{S}_h = \sigma_h(\mathcal{S}_1)$ for any d , which completes our proof. \square

We are now in a position to discuss the *approximation order* of local polyharmonic spline interpolation, according to Definition 3.1, for functions f in C^m .

To this end, regard for fixed $h > 0$ and $x \in \mathbb{R}^d$ the m -th order Taylor polynomial

$$T_{f,hx}^m(y) = \sum_{|\alpha| < m} \frac{1}{\alpha!} D^\alpha f(hx) (y - hx)^\alpha,$$

of $f \in C^m$ around hx , which yields the identity

$$f(hx) = T_{f,hx}^m(hx_i) - \sum_{0 < |\alpha| < m} \frac{1}{\alpha!} D^\alpha f(hx) (hx_i - hx)^\alpha, \quad \text{for all } 1 \leq i \leq n.$$

By using the representation (2.11) for s^h and the polynomial reproduction property (2.12), this immediately implies

$$f(hx) - s^h(hx) = \sum_{i=1}^n \lambda_i^h(hx) \left[T_{f,hx}^m(hx_i) - f(hx_i) \right].$$

Now due to Lemma 3.2, the *Lebesgue function*

$$\Lambda(x) = \sum_{i=1}^n |\lambda_i^h(hx)| = \sum_{i=1}^n |\lambda_i^1(x)|$$

is uniformly bounded in any local neighbourhood of the origin. Since we have

$$T_{f,hx}^m(hx_i) - f(hx_i) = \mathcal{O}(h^m), \quad h \rightarrow 0, \quad \text{for all } 1 \leq i \leq n,$$

this then implies

$$|f(hx) - s^h(hx)| = \mathcal{O}(h^m), \quad h \rightarrow 0.$$

Altogether, this proves the following

Theorem 3.3. *The approximation order of local polyharmonic spline interpolation, using $\phi_{d,k}$, with respect to C^m is $m = k - \lceil d/2 \rceil + 1$. \square*

We remark that the above Theorem 3.3 generalizes a previous result in [12] concerning the approximation order of local thin plate spline interpolation in the plane.

Corollary 3.4. *The approximation order of local thin plate spline interpolation, using $\phi_{2,2} = r^2 \log(r)$, with respect to C^2 is $m = 2$. \square*

4 Numerical Stability

This section is devoted to the construction of a numerically stable algorithm for the evaluation of polyharmonic spline interpolants. Recall that the stability of an algorithm always depends on the conditioning of the given problem. For a more general discussion on the relevant principles and concepts from error analysis, especially the *condition number* of a given *problem* versus the *stability* of a *numerical algorithm*, we recommend the textbook [13].

In order to briefly explain the conditioning of polyharmonic spline interpolation, let $U \subset \mathbb{R}^d$ denote a compact domain comprising $X = \{x_1, \dots, x_n\} \subset U$, the \mathcal{P}_m^d -unisolvant set of interpolation points. The condition number of polyharmonic spline interpolation w.r.t. the L_∞ -norm $\|\cdot\|_{L_\infty(U)}$ is given by the *Lebesgue constant*

$$\Lambda = \max_{x \in U} \sum_{i=1}^n |\lambda_i^1(x)|.$$

Note that a corresponding result for (univariate) polynomial interpolation is well-known from numerical analysis, see e.g. the textbook [6], where the arguments from there directly carry over to the situation of polyharmonic spline interpolation.

Now note that due to Lemma 3.2 the Lebesgue constant $\Lambda = \Lambda(U, X)$ is invariant under uniform scalings. But $\Lambda(U, X)$ is also invariant under rotations and translations. We summarize these observations as follows.

Theorem 4.5. *The condition number of polyharmonic spline interpolation is invariant under rotations, translations and uniform scalings.* \square

Now let us turn to the construction of a numerically stable algorithm for evaluating the polyharmonic spline interpolant s^h satisfying (2.6). To this end, we require that the given interpolation problem (2.6) is well-conditioned. Note that according to Theorem 4.5, this requirement depends on the geometry of the interpolation points X , but not on the scale h .

However, the spectral condition number of the matrix A_h depends on h . The following rescaling can be viewed as a simple way of preconditioning the matrix A_h for very small h . To this end, in order to evaluate the polyharmonic spline interpolant s^h satisfying (2.6), we prefer to work with the representation

$$s^h(hx) = \langle \beta_1(x), A_1^{-1} \cdot f_h \rangle, \quad (4.15)$$

which immediately follows from the identity (2.14) and the scale-invariance of the Lagrange basis, Lemma 3.2. Due to (4.15) we can evaluate s^h at hx by solving the linear system

$$A_1 \cdot \mathbf{b} = f_h. \quad (4.16)$$

The solution $\mathbf{b} \in \mathbb{R}^{n+q}$ in (4.16) then yields the coefficients of $s^h(hx)$ w.r.t. the basis functions in $\beta_1(x)$.

By working with the representation (4.15) for s^h instead of the one in (2.8), we can avoid solving the linear system (2.10). This is useful insofar as the linear system (2.10) is ill-conditioned for very small h , but well-conditioned for sufficiently large h . The latter relies on earlier results due to Narcowich and Ward [20], where it is shown that the spectral norm of the matrix Φ_h^{-1} is bounded above by a monotonically decreasing function of the minimal Euclidean distance between the points in hX . This in turns implies that one should, for the sake of numerical stability, avoid solving the system (2.10) directly for very small h . For further details on this, see [20] and the more general discussion provided by the recent paper [23] of Schaback.

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