Theoretical and computational aspects of multivariate interpolation with increasingly flat radial basis functions

Elisabeth Larsson* Bengt Fornberg**

June 10, 2003

Abstract

Multivariate interpolation of smooth data using smooth radial basis functions is considered. The behavior of the interpolants in the limit of nearly flat radial basis functions is studied both theoretically and numerically. Explicit criteria for different types of limits are given. Using the results for the limits, the dependence of the error on the shape parameter of the radial basis function is investigated. The mechanisms that determine the optimal shape parameter value are studied and explained through approximate expansions of the interpolation error.

Keywords: Radial basis function, RBF, interpolation, polynomial unisolvency

1 Introduction

The history of radial basis function (RBF) approximations goes back to 1968, when multiquadric RBFs were first used by Hardy to represent topographical surfaces given sets of sparse scattered measurements [1, 2]. Today, the literature on different aspects of RBF approximation is extensive. RBFs are used not only for interpolation or approximation of data sets [3], but also as tools for solving e.g., differential equations [4, 5, 6, 7, 8, 9, 10, 11]. However, their main strength remains the same: The ability to elegantly and accurately approximate scattered data without using any mesh. There have been some concerns about the computational cost and stability of the RBF methods, but many different viable approaches to overcome these difficulties have been proposed, see for example [12, 13, 14, 15, 16] and the references therein.

There are two main groups of radial basis functions, piecewise smooth and infinitely smooth. Some examples of both are given in Table 1. Typically, the piecewise smooth RBFs lead to an algebraic rate of convergence to the desired function as the number of points increase [17, 18], whereas the infinitely smooth RBFs yield a spectral or even faster rate of convergence [19, 20]. This is of course assuming that the desired function itself is smooth.

*Uppsala University, Department of Information Technology, Scientific Computing, Box 337, SE-751 05 Uppsala, Sweden (bette@it.uu.se). The work was supported by a postdoctoral grant from STINT, The Swedish Foundation for International Cooperation in Research and Higher Education and by a grant from The Swedish Research Council.

**University of Colorado, Department of Applied Mathematics, 526 UCB, Boulder, CO 80309, USA (fornberg@colorado.edu). The work was supported by NSF grants DMS-9810751 (VIGRE) and DMS-0309803.

Table 1: Some examples of radial basis functions.

Piecewise smooth RBFs	$\phi(r)$
Piecewise polynomial (R_n)	$\lvert r\rvert^n$, n odd
Thin Plate Spline (TPS_n)	$\lvert r\rvert^n \ln \lvert r\rvert$, n even
Infinitely smooth RBFs	$\phi(r)$
Multiquadric (MQ)	$\sqrt{1+r^2}$
Inverse multiquadric (IM)	$\frac{1}{\sqrt{1+r^2}}$
Inverse quadratic (IQ)	$\frac{1}{1+r^2}$
Gaussian (GA)	e^{-r^2}
Bessel (BE)	$J_0(2r)$

In this paper, we focus on interpolation of smooth data using RBFs even though some of the results may give insights also into cases were differential equations are solved. A typical interpolation problem has the following form: Given scattered data points $\underline{x}_j,\ j=1,\ldots,N$ and data $f_j = f(\underline{x}_j)$ find an interpolant

$$s(\underline{x}) = \sum_{j=1}^{N} \lambda_j\ \phi(\|\underline{x}-\underline{x}_j\|), \tag{1}$$

where $\underline{x}$ is a point in d space dimensions and $\|\cdot\|$ is the Euclidean norm. The interpolation conditions are

$$s(\underline{x}_i) = \sum_{j=1}^{N} \lambda_j\ \phi(\|\underline{x}_i-\underline{x}_j\|) = f_i, \quad i=1,\ldots,N.$$

This is summarized in a system of equations for the unknown coefficients λ_j,

$$A\underline{\lambda} = \underline{f}, \tag{2}$$

where $A_{ij} = \phi(\|\underline{x}_i-\underline{x}_j\|)$, $\underline{\lambda} = (\lambda_1,\ldots,\lambda_N)^T$, and $\underline{f} = (f_1,\ldots,f_N)^T$. We are interested in the case where $\phi(r)$ is infinitely smooth and belongs to the class of functions that can be expanded in even powers as

$$\phi(r) = a_0 + a_1 r^2 + a_2 r^4 + \ldots = \sum_{j=0}^{\infty} a_j r^{2j}. \tag{3}$$

Table 2 gives the expansion coefficients for the smooth RBFs in Table 1. All of these RBFs can be augmented by a shape parameter ε. This is done in such a way that $\phi(r)$ is replaced by $\phi(\varepsilon r)$. In previous studies [16, 11], we have found that for smooth data, the most accurate results are often obtained for very small values of ε both for interpolation problems and when solving elliptic partial differential equations. Small shape parameter values lead to almost flat RBFs, which in turn leads to severe ill-conditioning of the coefficient matrix A in (2). Hence, this is a region that has not been very well explored. However, even though the condition number of A is unbounded when $\varepsilon \to 0$, the limiting interpolant is often well behaved. In fact, it can be shown that the limit, if it exists, is a (multivariate) finite order

Table 2: Expansion coefficients for infinitely smooth RBFs.

RBF	Coefficients		
MQ	$a_0 = 1,$	$a_j = \frac{(-1)^{j+1}}{2j} \prod_{k=1}^{j-1} \frac{2k-1}{2k},$	$j = 1, \ldots$
IM	$a_0 = 1,$	$a_j = (-1)^j \prod_{k=1}^{j} \frac{2k-1}{2k},$	$j = 1, \ldots$
IQ		$a_j = (-1)^j,$	$j = 0, \ldots$
GA		$a_j = \frac{(-1)^j}{j!},$	$j = 0, \ldots$
BE		$a_j = \frac{(-1)^j}{(j!)^2},$	$j = 0, \ldots$

polynomial [21]. In one space dimension, under some mild assumptions on the RBF, the limit is the Lagrange interpolating polynomial if the points are distinct [22].

The aim of this paper is to extend the results of [22] to multivariate interpolation. Work in the same direction has been done independently by Schaback [23]. Some of the results that we present coincide with those in Schaback's paper. However, our approach is different from his and allows us to add information about the degree of the limiting polynomial and give precise conditions on the RBFs and the data points for different limit results. Furthermore, we can explain the behavior of the error in the interpolant for small ε and give reasons for why there is often a small nonzero optimal value of the shape parameter.

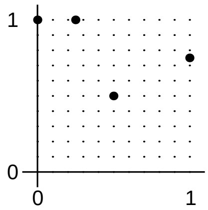
The outline of the paper is as follows. We start by presenting five examples, where the resulting limit interpolants are quite different. Section 3 contains definitions and background for the theorems concerning limit interpolants stated in Section 4. Section 5 contains the proofs of the theorems. Then, in light of the theoretical results, we go back to the examples and discuss them in Section 6. The ε-dependence of the error is considered in Section 7 and finally, we summarize the results in Section 8.

2 Examples of limit properties

In this section, we present a number of examples with different limit properties. All the examples are in two space dimensions, and clearly there are many more possibilities for the limits than in just one dimension, where we normally get the Lagrange interpolating polynomial. Explanations for the various results are given later in Sections 5 and 6.

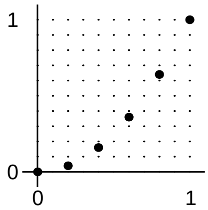
In each example, we use cardinal data for the interpolant. That is, the interpolant takes the value 1 at the first node point, $\underline{x}_1$, and is 0 at all other node points. We let x and y denote the spatial coordinates so that $\underline{x} = (x, y)$. The limits were computed analytically using Mathematica. Results are shown for the smooth RBFs defined in Table 1. In the tables of polynomial coefficients below, s is a factor that multiplies the entire polynomial.

Example 2.1 $\underline{x}_1 = (0, 1)$, $\underline{x}_2 = (\frac{1}{4}, 1)$, $\underline{x}_3 = (\frac{1}{2}, \frac{1}{2})$, $\underline{x}_4 = (1, \frac{3}{4})$
The points follow no specific pattern. All the limit interpolants are second order polynomials. The coefficients of the polynomials are given in the table below and clearly none of them are the same.



$\phi(r)$	s	1	x	y	x^2	xy	y^2
MQ	$\frac{1}{23}$	58	−97	−71	84	−16	36
IM	$\frac{1}{49}$	94	−191	−73	172	−48	28
IQ	$\frac{1}{31}$	56	−119	−37	108	−32	12
GA	$\frac{1}{13}$	18	−47	−1	44	−16	−4
BE	$\frac{1}{4}$	−1	−11	17	12	−8	−12

Example 2.2 $\underline{x}_k = \left(\frac{k-1}{5}, \left(\frac{k-1}{5}\right)^2\right), \quad k = 1, \ldots, 6.$

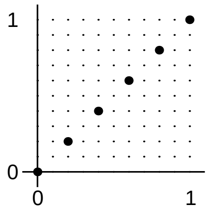


In this case, the points lie on a parabola. The degree of the limits is three. All of the limits are different even though there are some similarities. It is perhaps noteworthy that the GA limit is somewhat simpler than the other limits.

$\phi(r)$	s	1	x	y	x^2	xy	y^2	x^3	x^2y	xy^2	y^3
MQ	$\frac{1}{528}$	528	−5884	9606	13500	−39375	30375	−625	−1875	−2500	−3750
IM	$\frac{1}{720}$	720	−8028	21183	10375	−54125	41125	−625	−1875	−3750	−5000
IQ	$\frac{1}{816}$	816	−9100	26034	9750	−61500	46500	−625	−1875	−4375	−5625
GA	$\frac{1}{96}$	96	−1072	13726	0	−7375	5375	0	0	−625	−625
BE	$\frac{1}{144}$	144	−1620	13726	−7250	−12250	7250	625	1875	−1875	−625

Example 2.3 $\underline{x}_k = (\frac{k-1}{5}, \frac{k-1}{5}), \quad k = 1, \ldots, 6.$

Here, the points are on the line $x = y$. For MQ, IM, and IQ, the interpolants show divergence like $\mathcal{O}(1/\varepsilon^2)$. The coefficients of the divergent terms given below depend on the choice of RBF. Note that if the interpolant is evaluated on the line (which is in fact a 1D-case) the divergent terms disappear.



MQ: $\frac{1}{\varepsilon^2}\frac{625}{29568}\,(x-y)^2\,(18 - 7x - 7y)$

IM: $\frac{1}{\varepsilon^2}\frac{625}{2826368}\,(x-y)^2\,(666 - 355x - 355y)$

IQ: $\frac{1}{\varepsilon^2}\frac{625}{1559136}\,(x-y)^2\,(258 - 149x - 149y)$

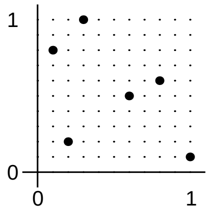
The GA and BE RBF do not lead to divergence. The limits are polynomials of degree five. The GA limit very nicely turns out to be the 1D Lagrange interpolation polynomial along the line in the variable $(x + y)$.

$$GA: \quad \frac{(10-5x-5y)}{10}\,\frac{(8-5x-5y)}{8}\,\frac{(6-5x-5y)}{6}\,\frac{(4-5x-5y)}{4}\,\frac{(2-5x-5y)}{2}$$

The BE limit does not factorize as nicely, but there is no divergence.

$$BE: \quad \frac{1}{192}(-6+5x+5y)\big(-32 + 156x + 156y + 130x^2 - 1240xy + 130y^2 - 600x^3 + 1200x^2y + 1200xy^2 - 600y^3 + 125x^4 + 500x^3y - 1750x^2y^2 + 500xy^3 + 125y^4\big)$$

Example 2.4 $\underline{x}_1 = (\frac{1}{10}, \frac{4}{5})$, $\underline{x}_2 = (\frac{1}{5}, \frac{1}{5})$, $\underline{x}_3 = (\frac{3}{10}, 1)$, $\underline{x}_4 = (\frac{3}{5}, \frac{1}{2})$, $\underline{x}_5 = (\frac{4}{5}, \frac{3}{5})$, $\underline{x}_6 = (1, \frac{1}{10})$.

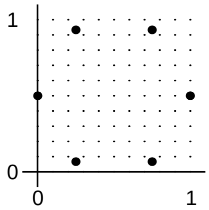


These six points do not follow any particular pattern. The MQ, IM, IQ, and GA RBF interpolants all have the same limit, $p(x)$, which is the unique second order polynomial interpolating the cardinal data. The BE RBF gives a different limit, which is a third order polynomial.

$$p(x) = \frac{1}{28274}(-7711 - 81420x + 132915y + 82300x^2 - 55450xy - 91550y^2)$$

$$\begin{aligned} \textit{BE:} \quad -\frac{1}{1017250518}(&-354545067 - 2047021330x + 4593056085y \\ &+2554383300x^2 - 4166831700xy - 2554383300y^2 \\ &-310763000x^3 + 1319845500x^2y + 932289000xy^2 \\ &-439948500y^3) \end{aligned}$$

Example 2.5 $\underline{x}_k = \frac{1}{2}\left(\cos\left(\frac{(k-1)\pi}{3}\right) + 1, \sin\left(\frac{(k-1)\pi}{3}\right) + 1\right), \quad k = 1, \ldots, 6.$



The points lie on a circle. There is no unique interpolating polynomial. Nevertheless, all RBFs, including the BE RBF have the same limit interpolant of degree three,

$$p(x) = \frac{1}{6}(1 - 4x - 4y - 4x^2 + 24xy + 4y^2 + 8x^3 - 24xy^2).$$

3 Definitions

This section contains definitions for multi-index notation, gives some properties of polynomial interpolation, and looks at expansions of smooth RBFs. This is all needed for the theorems in the following section and their proofs.

3.1 Multi-index notation

Since we consider multivariate interpolation in any number of dimensions, multi-indices greatly simplify awkward expressions. We need some basic operations and some different types of multi-index sets.

Definition 3.1 *Let $j = (j_1, j_2, \ldots, j_d)$, where each j_n is a non-negative integer, be a multi-index. Then define the following properties for multi-indices j and k.*

(a) The absolute value $|j| = \sum_{n=1}^{d} j_n$.

(b) Addition, and multiplication by scalars, $m = \alpha j + \beta k = (\alpha j_1 + \beta k_1, \ldots, \alpha j_d + \beta k_d)$, is allowed if the result is a multi-index.

(c) *Polynomial ordering of a sequence of multi-indices is determined in the following way: The multi-index j comes before k in the sequence if $|j| < |k|$, or if $|j| = |k|$, $j_n = k_n$, $n = 1, \dots, p$ and $j_{p+1} > k_{p+1}$.*

(d) *If $\underline{x} = (x_1, x_2, \dots, x_d)$ is a point in d-dimensional space then $\underline{x}^j = x_1^{j_1} x_2^{j_2} \cdots x_d^{j_d}$.*

(e) *Derivatives can be expressed with multi-indices as $\phi^{(j)}(\underline{x}) = \frac{\partial^{|j|}\phi(\underline{x})}{\partial x_1^{j_1} \cdots \partial x_d^{j_d}}$.*

(f) *The factorial of a multi-index is $j! = j_1! \cdots j_d!$.*

(g) *The multi-indices j and k have the same parity if j_n and k_n have the same parity for $n = 1, \dots, d$.*

Definition 3.2 *Let J_K, where $K \geq 0$, be the polynomially ordered sequence of all multi-indices j such that $|j| \leq K$. Let $J_K(n)$ denote the nth multi-index in the sequence.*

Definition 3.3 *Let $I_{p,K}$, where $0 \leq p \leq d$ and $K \geq 0$, be the polynomially ordered sequence of all multi-indices j such that $j_1, \dots, j_p$ are odd numbers, $j_{p+1}, \dots, j_d$ are even numbers, and $|j| \leq K$. Let $I_{p,K}(n)$ denote the nth multi-index in the sequence.*

Definition 3.4 *Let $I_{p,K}^i$ be the ith unique permutation of $I_{p,K}$. Each set $I_{p,K}$ has $\binom{d}{p}$ unique permutations. A permutation of a set is done in such a way that the same permutation is applied to each multi-index. The order of the multi-indices in the original set is retained for the new set. Unique permutations lead to sets that are distinguishable from each other.*

Example 3.1 *The set $I_{1,3} = \{(1,0,0), (3,0,0), (1,2,0), (1,0,2)\}$ for $d = 3$ has three unique permutations $I_{1,3}^1 = I_{1,3}$, $I_{1,3}^2 = \{(0,1,0), (0,3,0), (2,1,0), (0,1,2)\}$, and $I_{1,3}^3 = \{(0,0,1), (0,0,3), (0,2,1), (2,0,1)\}$.*

Definition 3.5 *Let I_{2m}^j be the polynomially ordered set of all multi-indices k such that $|j + k| = 2m$, and j and k have the same parity.*

Example 3.2 *The set $I_4^{(0,0)} = \{(4,0), (2,2), (0,4)\}$ and the set $I_4^{(1,0)} = \{(3,0), (1,2)\}$.*

3.2 Polynomial spaces and unisolvency

As mentioned before, the limit of an RBF interpolant as the shape parameter goes to zero must be polynomial if it exists [21]. In the following sections, it will become clear that there are close parallels between plain polynomial interpolation and interpolation in the limit of flat RBFs. The following definitions and relations are useful in this context.

Definition 3.6 *Let $P_{K,d}$ be the space of all polynomials of degree $\leq K$ in d spatial dimensions. The dimension of $P_{K,d}$ is given by*

$$N_{K,d} = \binom{K+d}{K}. \tag{4}$$

A basis for $P_{K,d}$ is given by $\{p_i(\underline{x})\}_{i=1}^{N_{K,d}}$, where $p_i(\underline{x}) = \underline{x}^{J_K(i)}$. Table 3 shows some examples of the values of $N_{K,d}$. A relation that may be useful is that $N_{K,d} - N_{K-1,d} = N_{K,d-1}$.

Table 3: The dimension, $N(K,d)$, of the space of all polynomials of degree $\leq K$ in d variables.

K	$d=1$	$d=2$	$d=3$
0	1	1	1
1	2	3	4
2	3	6	10
3	4	10	20
4	5	15	35
5	6	21	56
6	7	28	84
7	8	36	120
8	9	45	165

A property that is connected with the distribution of the data points is polynomial unisolvency [24]. The following theorem gives necessary and sufficient conditions for unisolvency. The proof is straightforward and will not be given here.

Theorem 3.1 *Let $\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_n$ be n point locations, and let $p_1(\underline{x}), p_2(\underline{x}), \ldots, p_n(\underline{x})$ be n linearly independent polynomials. Then $\{\underline{x}_i\}$ is unisolvent with respect to $\{p_i(\underline{x})\}$, i.e., there is a unique linear combination $\sum \beta_j p_j(\underline{x})$ which interpolates any given data over the point set, if and only if det$(P) \neq 0$, where*

$$P = \begin{pmatrix} p_1(\underline{x}_1) & p_2(\underline{x}_1) & \cdots & p_n(\underline{x}_1) \\ p_1(\underline{x}_2) & p_2(\underline{x}_2) & \cdots & p_n(\underline{x}_2) \\ \vdots & \vdots & & \vdots \\ p_1(\underline{x}_n) & p_2(\underline{x}_n) & \cdots & p_n(\underline{x}_n) \end{pmatrix}.$$

Corollary 3.1 *If* $\det(P) = 0$*, then the nullspace of P describes all the possible ambiguities in the resulting interpolant of the specified form.*

Definition 3.7 *Let $N_{K-1,d} < N \leq N_{K,d}$ and let $\{\underline{x}_i\}_{i=1}^N$ be a set of distinct points that is non-unisolvent with respect to any choice of N linearly independent basis functions from $P_{K,d}$. There is a smallest integer $M > K$ such that the matrix P, constructed from a basis in $P_{M,d}$ and the point set under consideration, has exactly rank N. We can form a minimal non-degenerate basis $\{p_i(\underline{x})\}_{i=1}^N$, using a subset of the basis in $P_{M,d}$ corresponding to linearly independent columns in P. The degree of the minimal non-degenerate basis is M.*

Corollary 3.2 *If $N_{K-1,d} < N \leq N_{K,d}$ and if $\{\underline{x}_i\}_{i=1}^N$ is unisolvent with respect to any set of N linearly independent polynomials from $P_{K,d}$, then*

(i) if $N = N_{K,d}$ there is a unique *interpolating polynomial of degree K for any given data on the point set,*

(ii) if $N < N_{K,d}$ there is an interpolating polynomial of degree K for any given data on the point set for each choice of N linearly independent basis functions.

If the point set $\{\underline{x}_i\}_{i=1}^N$ is non-unisolvent and the degree of the minimal non-degenerate basis is M, then *(iii) there is an interpolating polynomial of degree M for any given data on the point set, for each choice of a minimal non-degenerate basis.*

3.3 Expansions of RBFs

The class of RBFs that we consider has expansions in r of type (3). For one particular basis function in the linear combination forming the interpolant (1) we have

$$\phi(\|\underline{x}-\underline{x}_k\|) = \phi(r_k) = a_0 + a_1 r_k^2 + a_2 r_k^4 + a_3 r_k^6 + \dots$$

Viewing the RBF as a polynomial of infinite degree, we need to express the expansion in powers of $\underline{x}$. We start with considering just one term. The coefficient of $\underline{x}^j$ in r_k^{2m} ($|j| \le 2m$) is

$$r_k^{2m}\big|_{\underline{x}^j} = \sum_{\ell \in I_{2m}^j} (-1)^{|j|} \frac{m!}{(\frac{j+\ell}{2})!} \frac{(j+\ell)!}{j!\ \ell!} \underline{x}_k^\ell. \tag{5}$$

If we collect all contributions with power j in $\underline{x}$ from the basis function we get

$$\phi(\|\underline{x}-\underline{x}_k\|)\big|_{\underline{x}^j} = \sum_{m=\left|\lfloor \frac{j+1}{2} \rfloor\right|}^{\infty} a_m \sum_{\ell \in I_{2m}^j} (-1)^{|j|} \frac{m!}{(\frac{j+\ell}{2})!} \frac{(j+\ell)!}{j!\ \ell!} \underline{x}_k^\ell, \tag{6}$$

where if for example $j = (1,2,2)$, the sum over m starts at $\left|\left\lfloor \frac{(2,3,3)}{2} \right\rfloor\right| = 3$. Note that there is a certain system in how the coefficients are formed. For example, the coefficient of $\underline{x}^j$ for any j with all even components only contain $\underline{x}_k^\ell$ for ℓ with all even components. There is a decoupling of powers with different parity.

In the theorems, certain subsets of these coefficients are important. We need the matrices defined below, which consist of coefficients for powers with the same parity and with the total powers of $\underline{x}$ and $\underline{x}_k$ both restricted to be $\le K$.

Definition 3.8 *Let the elements of the matrix $A_{p,K}$ be defined by*

$$A_{p,K}(r,c) = a_m (-1)^{|j|} \frac{m!}{(\frac{j+k}{2})!} \frac{(j+k)!}{j!k!} \tag{7}$$

where $j = I_{p,K}(r)$, $k = I_{p,K}(c)$, and $2m = |j+k|$. The size of the matrix is determined by the number of elements in $I_{p,K}$.

To illustrate what the definition leads to, we give two examples of index sets and matrices. The first example for the one dimensional case gives the matrices that were derived in [22].

Example 3.3 *In one space dimension, (7) is reduced to*

$$A_{p,K}(r,c) = a_m (-1)^j \begin{pmatrix} j+k \\ j \end{pmatrix}.$$

For $K=5$, we get $I_{0,5} = \{(0),(2),(4)\}$ and $I_{1,5} = \{(1),(3),(5)\}$, leading to the matrices

$$A_{0,5} = \begin{pmatrix} a_0 & a_1 & a_2 \\ a_1 & 6a_2 & 15a_3 \\ a_2 & 15a_3 & 70a_4 \end{pmatrix}, \quad A_{1,5} = -\begin{pmatrix} 2a_1 & 4a_2 & 6a_3 \\ 4a_2 & 20a_3 & 56a_4 \\ 6a_3 & 56a_4 & 252a_5 \end{pmatrix}$$

Example 3.4 *In three space dimensions, (7) instead becomes*

$$A_{p,K}(r,c) = \frac{a_m(-1)^{|j|}m!}{(\frac{j_1+k_1}{2})!(\frac{j_2+k_2}{2})!(\frac{j_3+k_3}{2})!}\begin{pmatrix} j_1+k_1 \\ j_1 \end{pmatrix}\begin{pmatrix} j_2+k_2 \\ j_2 \end{pmatrix}\begin{pmatrix} j_3+k_3 \\ j_3 \end{pmatrix},$$

For $K=5$, *we get the four multi-index sets*
$I_{0,5} = \{(0,0,0),(2,0,0),(0,2,0),(0,0,2),(4,0,0),(2,2,0),(2,0,2),(0,4,0),(0,2,2),(0,0,4)\}$,
$I_{1,5} = \{(1,0,0),(3,0,0),(1,2,0),(1,0,2),(5,0,0),(3,2,0),(3,0,2),(1,4,0),(1,2,2),(1,0,4)\}$,
$I_{2,5} = \{(1,1,0),(3,1,0),(1,3,0),(1,1,2)\}$, *and*
$I_{3,5} = \{(1,1,1),(3,1,1),(1,3,1),(1,1,3)\}$.
The four corresponding matrices are

$$A_{0,5} = \left(\begin{array}{c|ccc|cccccc}
a_0 & a_1 & a_1 & a_1 & a_2 & 2a_2 & 2a_2 & a_2 & 2a_2 & a_2 \\ \hline
a_1 & 6a_2 & 2a_2 & 2a_2 & 15a_3 & 18a_3 & 18a_3 & 3a_3 & 6a_3 & 3a_3 \\
a_1 & 2a_2 & 6a_2 & 2a_2 & 3a_3 & 18a_3 & 6a_3 & 15a_3 & 18a_3 & 3a_3 \\
a_1 & 2a_2 & 2a_2 & 6a_2 & 3a_3 & 6a_3 & 18a_3 & 3a_3 & 18a_3 & 15a_3 \\ \hline
a_2 & 15a_3 & 3a_3 & 3a_3 & 70a_4 & 60a_4 & 60a_4 & 6a_4 & 12a_4 & 6a_4 \\
2a_2 & 18a_3 & 18a_3 & 6a_3 & 60a_4 & 216a_4 & 72a_4 & 60a_4 & 72a_4 & 12a_4 \\
2a_2 & 18a_3 & 6a_3 & 18a_3 & 60a_4 & 72a_4 & 216a_4 & 12a_4 & 72a_4 & 60a_4 \\
a_2 & 3a_3 & 15a_3 & 3a_3 & 6a_4 & 60a_4 & 12a_4 & 70a_4 & 60a_4 & 6a_4 \\
2a_2 & 6a_3 & 18a_3 & 18a_3 & 12a_4 & 72a_4 & 72a_4 & 60a_4 & 216a_4 & 60a_4 \\
a_2 & 3a_3 & 3a_3 & 15a_3 & 6a_4 & 12a_4 & 60a_4 & 6a_4 & 60a_4 & 70a_4
\end{array}\right),$$

$$A_{1,5} = -\left(\begin{array}{c|ccc|cccccc}
2a_1 & 4a_2 & 4a_2 & 4a_2 & 6a_3 & 12a_3 & 12a_3 & 6a_3 & 12a_3 & 6a_3 \\ \hline
4a_2 & 20a_3 & 12a_3 & 12a_3 & 56a_4 & 80a_4 & 80a_4 & 24a_4 & 48a_4 & 24a_4 \\
4a_2 & 12a_3 & 36a_3 & 12a_3 & 24a_4 & 144a_4 & 48a_4 & 120a_4 & 144a_4 & 24a_4 \\
4a_2 & 12a_3 & 12a_3 & 36a_3 & 24a_4 & 48a_4 & 144a_4 & 24a_4 & 144a_4 & 120a_4 \\ \hline
6a_3 & 56a_4 & 24a_4 & 24a_4 & 252a_5 & 280a_5 & 280a_5 & 60a_5 & 120a_5 & 60a_5 \\
12a_3 & 80a_4 & 144a_4 & 48a_4 & 280a_5 & 1200a_5 & 400a_5 & 600a_5 & 720a_5 & 120a_5 \\
12a_3 & 80a_4 & 48a_4 & 144a_4 & 280a_5 & 400a_5 & 1200a_5 & 120a_5 & 720a_5 & 600a_5 \\
6a_3 & 24a_4 & 120a_4 & 24a_4 & 60a_5 & 600a_5 & 120a_5 & 700a_5 & 600a_5 & 60a_5 \\
12a_3 & 48a_4 & 144a_4 & 144a_4 & 120a_5 & 720a_5 & 720a_5 & 600a_5 & 2160a_5 & 600a_5 \\
6a_3 & 24a_4 & 24a_4 & 120a_4 & 60a_5 & 120a_5 & 600a_5 & 60a_5 & 600a_5 & 700a_5
\end{array}\right),$$

$$A_{2,5} = \left(\begin{array}{c|ccc}
8a_2 & 24a_3 & 24a_3 & 24a_3 \\ \hline
24a_3 & 160a_4 & 96a_4 & 96a_4 \\
24a_3 & 96a_4 & 160a_4 & 96a_4 \\
24a_3 & 96a_4 & 96a_4 & 288a_4
\end{array}\right), \quad A_{3,5} = -\left(\begin{array}{c|ccc}
48a_3 & 192a_4 & 192a_4 & 192a_4 \\ \hline
192a_4 & 1600a_5 & 960a_5 & 960a_5 \\
192a_4 & 960a_5 & 1600a_5 & 960a_5 \\
192a_4 & 960a_5 & 960a_5 & 1600a_5
\end{array}\right).$$

4 Theorems concerning limits

Now we have enough background to state some theorems about interpolants in the limit $\varepsilon \to 0$. We use the cases (i), (ii), and (iii) from Corollary 3.2 to categorize the data points and we require the RBF $\phi(r)$ to fulfill the following conditions:

(I) The Taylor expansion of $\phi(r)$ is of type (3).

(II) The matrix A in system (2) is non-singular in the interval $0 < \varepsilon \le R$, for some $R > 0$.

(III) The matrices $A_{p,J}$ from Definition 3.8 are non-singular for $0 \le p \le d$ and $0 \le J \le K$ when the expansion coefficients for $\phi(r)$ are used.

Theorem 4.1 *Consider the interpolation problem (1)–(2). If the node points $\{\underline{x}_i\}$ are of type (i) and the RBF satisfies (I)–(III), then the limit of the RBF interpolant as the shape parameter $\varepsilon \to 0$ is the* unique *interpolating polynomial $P(\underline{x})$ of degree K to the given data. For $\varepsilon > 0$, the interpolant has the form*

$$s(\underline{x}, \varepsilon) = P(\underline{x}) + \varepsilon^2 p_1(\underline{x}) + \varepsilon^4 p_2(\underline{x}) + \cdots,$$

where $p_j(\underline{x})$ are polynomials of degree $K+2j$. If the data is such that $P(\underline{x})$ becomes of degree $K - Q$ then the interpolant takes the form

$$s(\underline{x}, \varepsilon) = P(\underline{x}) + \varepsilon^{2r+2} p_{r+1}(\underline{x}) + \varepsilon^{2r+4} p_{r+2}(\underline{x}) + \cdots,$$

where $r = \lfloor \frac{Q}{2} \rfloor$ and $p_{r+j}(\underline{x})$ are polynomials of degree $K + 2j - 1$ if Q is odd and $K + 2j$ if Q is even.

Theorem 4.2 *Consider the interpolation problem (1)–(2). If the node points $\{\underline{x}_i\}$ are of type (ii) and the RBF satisfies (I)–(III), then the limit of the RBF interpolant as the shape parameter $\varepsilon \to 0$ is* a *polynomial $P(\underline{x})$ of degree K that interpolates the given data. The exact polynomial depends on the choice of RBF. The form of the interpolant is the same as in the previous case and for low degree data, we get the same kind of change in the expansion.*

Theorem 4.3 *Consider the interpolation problem (1)–(2). If the node points $\{\underline{x}_i\}$ are of type (iii) and the RBF satisfies (I)–(III), then the limit of the RBF interpolant as the shape parameter $\varepsilon \to 0$, if it exists, is* a *polynomial $P(\underline{x})$ of degree M that interpolates the given data. For $\varepsilon > 0$ the interpolant has the form*

$$s(\underline{x}, \varepsilon) = P(\underline{x}) + \varepsilon^2 p_1(\underline{x}) + \varepsilon^4 p_2(\underline{x}) + \cdots,$$

where $p_j(\underline{x})$ are polynomials of degree $M + 2j$.

If the limit does not exist, i.e., there are divergent terms, the interpolant takes the form

$$s(\underline{x}, \varepsilon) = \varepsilon^{-2z} p_z(\underline{x}) + \varepsilon^{-2z+2} p_{z-1}(\underline{x}) + \cdots + \varepsilon^{-2} p_1(\underline{x}) + P(\underline{x}) + \mathcal{O}(\varepsilon^2),$$

where $z = \left\lfloor \frac{M-N_0}{2} \right\rfloor$ and N_0 is the degree of the lowest order polynomial in the nullspace of the matrix P corresponding to a basis of $P_{M,d}$. The polynomials $p_j(\underline{x})$ have degree $M - 2j$ and are in the nullspace of P. Note that some of the polynomials p_j may be zero, that is, the divergence may be of lower order than ε^{-2z}, which is the worst possible case. This depends on the specific point distribution.

Also here, if the data is such that $P(\underline{x})$ becomes of degree $M - Q$, the degrees of the polynomials $p_j(\underline{x})$ are lowered by the same amount. The number of possible divergent terms is then lowered to $z = \left\lfloor \frac{M-Q-N_0}{2} \right\rfloor$.

Remark: If we could discard the divergent terms, we would get a limit that makes sense also with the non-unisolvent point sets. This may be possible to achieve, at least in some cases, using the Contour-Padé approach described in [16]. Furthermore, in [21], we conjectured that the divergent terms are always zero if the GA RBF is used. Schaback [23] showed that the limit when using GA RBFs is least in a certain sense.

Corollary 4.1 *If Theorem 4.1 or 4.2 holds, then the coefficients of the linear combination in the interpolant, λ_j, $j = 1, \dots, N$, grow as ε^{-2K} as $\varepsilon \to 0$. If instead Theorem 4.3 holds, the growth is of order ε^{-2M}.*

Conjecture 4.1 *Condition (III) holds for all commonly used RBFs such as MQ, IM, IQ and GA.*

We have no proof for this except that we have found it to be true for all cases that we have been able to test. For basis functions that fail condition (III), it is hard to give any general guidelines as to what happens as the shape parameter $\varepsilon \to 0$. The limit of the RBF interpolant may or may not exist and in general, the degree of the limit if it exists is different from what a basis function that fulfills the condition would give. This type of function seems to be less prone to divergence in non-unisolvent cases, but we have not found any other clear advantages so far.

5 Proofs

The proofs for the theorems are constructive in nature and give some insights that we can use in the discussion of errors in the following section. They are therefore presented here in quite a lot of detail. The approach is similar to the method used in [22], but is here extended to any number of space dimensions.

5.1 General ingredients in the proofs

We consider the interpolation problem (1)–(2) with node points $\underline{x}_k$, $k = 1, \dots, N$, in d dimensions, where $N_{K-1,d} < N \le N_{K,d}$.

From condition (I), the basis function $\phi(r)$ has an expansion in even powers of r. If we include a shape parameter ε, we have

$$\phi(\varepsilon r) = a_0 + \varepsilon^2 a_1 r^2 + \varepsilon^4 a_2 r^4 + \cdots = \sum_{j=0}^{\infty} \varepsilon^{2j} a_j r^{2j}. \tag{8}$$

Each entry in the matrix A of the system (2) can be expanded in even powers of ε as above. Condition (II) says that A is non-singular for an interval $0 < \varepsilon \le R$. Since, for this range of ε-values, the system can be solved by Cramer's rule, each element in $\underline{\lambda}$ must be a rational function of ε^2. This means that for some finite q we have

$$\underline{\lambda} = \varepsilon^{-2K}(\varepsilon^{-2q}\underline{\lambda}_{-q} + \cdots + \underline{\lambda}_0 + \varepsilon^2\underline{\lambda}_1 + \cdots). \tag{9}$$

Let the discrete moments of $\underline{\lambda}_r = (\lambda_{1,r}, \dots, \lambda_{N,r})^T$ be defined in the following way

$$\sigma_r^{(\ell)} = \sum_{k=1}^{N} \lambda_{k,r} \underline{x}_k^{\ell}, \quad r = -q, \dots, \infty. \tag{10}$$

If we pick N linearly independent polynomials $p_i(\underline{x}) = \underline{x}^{\ell_i}$ and form a matrix T, where $t_{ij} = p_j(\underline{x}_i)$ (as for P in Theorem 3.1), in such a way that T is nonsingular, then

$$\underline{\sigma}_r = T^T \underline{\lambda}_r, \quad r = -q, \dots, \infty, \tag{11}$$

where $\underline{\sigma}_r = (\sigma_r^{(\ell_1)}, \dots, \sigma_r^{(\ell_N)})^T$. When $\underline{\sigma}_r$ is known, we can compute any other moment $\sigma_r^{(\ell)}$ through

$$\sigma_r^{(\ell)} = \sum_{k=1}^{N} \lambda_{k,r} \underline{x}_k^{\ell} \equiv \underline{v}^T \underline{\lambda}_r = \underline{v}^T T^{-T} \underline{\sigma}_r. \tag{12}$$

Combining the two expansions (8) and (9) and inserting them into the form of the interpolant (1) yields

$$s(\underline{x}, \varepsilon) = \sum_{k=1}^{N} \lambda_k \phi(\|\underline{x} - \underline{x}_k\|) = \varepsilon^{-2K}(\varepsilon^{-2q} P_{-q}(\underline{x}) + \cdots + \varepsilon^{2K} P_K(\underline{x}) + \cdots), \tag{13}$$

where $P_{-q+s} = \sum_{m=0}^{s} a_m \sum_{k=1}^{N} \lambda_{k,-q+s-m} r_k^{2m}$. We need the coefficient of each polynomial term. If we use (5) as we did for (6) and also apply definition (10), we get

$$P_{-q+s}|_{\underline{x}^j} = \sum_{m=|\lfloor \frac{j+1}{2} \rfloor|}^{s} a_m \sum_{\ell \in I_{2m}^j} (-1)^{|j|} \frac{m!}{(\frac{j+\ell}{2})!} \frac{(j+\ell)!}{j!\,\ell!} \sigma_{-q+s-m}^{(\ell)}.$$

The highest degree terms that can contribute to P_{-q+s} have $|j| = 2s$ and we can express the polynomial as

$$P_{-q+s}(\underline{x}) = \sum_{j \in J_{2s}} \left(\sum_{m=|\lfloor \frac{j+1}{2} \rfloor|}^{s} a_m \sum_{\ell \in I_{2m}^j} (-1)^{|j|} \frac{m!}{(\frac{j+\ell}{2})!} \frac{(j+\ell)!}{j!\,\ell!} \sigma_{-q+s-m}^{(\ell)} \right) \underline{x}^j. \tag{14}$$

Note that some of the terms with total power $2s$ are usually missing from the polynomial. In the expression this shows only through the fact that the sum over m is empty in those cases. A close inspection of the polynomial terms reveals that:

- The coefficients of $\underline{x}^j$ in P_{-q+s}, where $2s - |j| = J$ all involve the same discrete moments $\sigma_{-q+r}^{(\ell)}$ with $2r + |\ell| = J$.
- $J = 0$ corresponds to the highest order terms in each polynomial, $J = 1$ corresponds to the next to highest order terms in each polynomial, and so on for larger J.
- For each J the number of moments that are involved is finite, since $r \geq 0$, $|\ell| \geq 0$, and $2r + |\ell| = J$. If we can compute these moments, we can also find the coefficients of the corresponding terms in *every* polynomial P_{-q+s}.

Definition 5.1 *The vector* $\underline{\sigma}^i_{p,J}$ *has elements* $\sigma^{(\ell)}_{-q+r}$*, where for the kth element,* $\ell = I^i_{p,J}(k)$ *and* $r = (J - |\ell|)/2$.

Definition 5.2 *The elements of the vector* $\underline{p}^i_{p,J}$ *are the coefficients of* $\underline{x}^j$ *in* P_{-q+s}*, where for the kth element* $j = I^i_{p,J}(k)$ *and* $s = (J + |j|)/2$*. This means that* $J/2 \le s \le J$ *holds for all elements in the vector.*

Example 5.1 *In two dimensions, the vector of moments*
$\underline{\sigma}^1_{0,4} = (\sigma^{(0,0)}_{-q+2}, \sigma^{(2,0)}_{-q+1}, \sigma^{(0,2)}_{-q+1}, \sigma^{(4,0)}_{-q}, \sigma^{(2,2)}_{-q}, \sigma^{(0,4)}_{-q})^T$ *and the corresponding vector*
$\underline{p}^1_{0,4} = (P_{-q+2}|_{\underline{x}^{(0,0)}}, P_{-q+3}|_{\underline{x}^{(2,0)}}, P_{-q+3}|_{\underline{x}^{(0,2)}}, P_{-q+4}|_{\underline{x}^{(4,0)}}, P_{-q+4}|_{\underline{x}^{(2,2)}}, P_{-q+4}|_{\underline{x}^{(0,4)}},)^T$.

With the matrices from Definition 3.8 and the vectors defined above, we can form a sequence of systems of equations for the discrete moments,

$$A_{p,J}\underline{\sigma}^i_{p,J} = \underline{p}^i_{p,J}, \tag{15}$$

where p and J have the same parity, $0 \le p \le d$, $i = 1, \ldots, \begin{pmatrix} d \\ p \end{pmatrix}$, and $J = 0, 1, \ldots, \infty$. Since condition (III) holds for $\phi(r)$, all of the systems are nonsingular and we have a complete description of the relation between the discrete moments and the polynomials P_{-q+s}. With knowledge of the polynomial coefficients, the systems in (15) can be used directly for determining the moments.

Following condition (II), there is a whole range of ε-values for which we get a well defined interpolant to the data. If we relate this to the expansion (13), we see that the polynomial multiplying ε^0 must interpolate the data and all other polynomials must be zero at the data locations. That is, we get the following conditions

$$\begin{array}{ll} P_K & \text{interpolates the data at the } N \text{ node points} \\ P_j, \quad j \neq K & \text{interpolate 0 at the } N \text{ node points.} \end{array} \tag{16}$$

All of the above holds for each type of point set. In the following three subsections, we go through the specifics for each case.

5.2 Proof of Theorem 4.1

The point set is of type (i), meaning that the number of points equal $N_{K,d}$ for some K and the point set is unisolvent with respect to any basis in $P_{K,d}$. Accordingly, relation (11) holds for the basis $\{\underline{x}^{J_K(i)}\}_{i=1}^{N_{K,d}}$.

We know that the degree of $P_{-q+s}(\underline{x})$ is at most $2s$. Because of the unisolvency, any polynomial with degree $\le K$ that interpolates zero at N points must be identically zero. Following condition (16), this includes at least the following polynomials

$$P_{-q} = P_{-q+1} = \cdots = P_{-q+\lfloor \frac{K+1}{2} \rfloor -1} = 0.$$

We can immediately go ahead and solve all systems in (15) with $J \le \lfloor \frac{K+1}{2} \rfloor - 1$, since their right hand sides are all zero. Because the coefficient matrices are nonsingular, the solutions are that all involved $\underline{\sigma}^i_{p,J} = \underline{0}$. Now, remember that the moments for $J = 0$ determine the highest order coefficients in each P_{-q+s}. These will therefore all be zero, and the degree of every polynomial is reduced by one. This occurs again for every J and after $\lfloor\frac{K+1}{2}\rfloor$ steps we have that the degree of P_{-q+s} is at most $2s-\lfloor\frac{K+1}{2}\rfloor$. That is, there are now more polynomials with degree lower than K, which have to be zero. In fact, if we take into account that the degree continues to be lowered by one for each new J, we finally get

$$P_{-q} = P_{-q+1} = \ldots = P_{-q+K-1} = 0.$$

The degree of P_{-q+K} is K and we have a choice: either $P_{-q+K} = P_K$ and interpolates the data or it is zero at N points. Assume that $q > 0$ so that $P_{-q+K} \neq P_K$. Then the polynomial is zero at the data points, which means that it must be identically zero and we can solve also the systems for $J = K$. If we look at the discrete moments that have then been determined, we find that

$$\begin{array}{lcll} \sigma^{(\ell)}_{-q} & = & 0, & |\ell| \leq K, \\ \sigma^{(\ell)}_{-q+1} & = & 0, & |\ell| \leq K-2, \\ \sigma^{(\ell)}_{-q+2} & = & 0, & |\ell| \leq K-4, \\ \vdots & & & \vdots \\ \sigma^{(\ell)}_{-q+\lfloor\frac{K}{2}\rfloor} & = & 0, & |\ell| \leq K - 2\left\lfloor\frac{K}{2}\right\rfloor, \end{array}$$

but then following (11), $\underline{\lambda}_{-q} = \underline{0}$ and we could have omitted that term in the expansion (9). We have a contradiction. We must have $q = 0$ and the expansion of the coefficients of the interpolant has the following form

$$\underline{\lambda} = \varepsilon^{-2K}\underline{\lambda}_0 + \varepsilon^{-2K+2}\underline{\lambda}_1 + \cdots.$$

As a byproduct this tells us that the smallest eigenvalue of A is of order ε^{2K}, since $\underline{\lambda} = A^{-1}\underline{f}$ for any data vector f. This was proved by Schaback [23] and he also gives the magnitudes in ε for all of the eigenvalues.*

Because the lower order polynomials are all forced to be zero by condition (16), the interpolant becomes

$$s(\underline{x},\varepsilon) = P_K(\underline{x}) + \varepsilon^2 P_{K+1}(\underline{x}) + \varepsilon^4 P_{K+2}(\underline{x}) + \cdots.$$

Unisolvency ensures that P_K is the unique interpolating polynomial to the given data. The degree of $P_{K+j} = 2(K+j) - K = K + 2j$.

The data may be such that the interpolating polynomial P_K becomes of degree $K-Q$. In this case, also the systems of equations for $J = K, \ldots, K+Q-1$ have zero right hand sides. This corresponds to a lowering of the degree of each polynomial by Q, i.e., P_{K+j} has degree $K+2j-Q$. Condition (16) holds for all the polynomials P_{K+j} and if Q is large enough to bring the degree down to K or less for a polynomial, then that polynomial is zero. We get a modified expression for the interpolant

$$s(\underline{x},\varepsilon) = P_K(\underline{x}) + \varepsilon^{2r+2} P_{K+r+1}(\underline{x}) + \varepsilon^{2r+4} P_{K+r+2}(\underline{x}) + \cdots,$$

where $r = \lfloor\frac{Q}{2}\rfloor$. The degree of P_{K+r+j} is $K+2j-1$ if Q is odd and $K+2j$ if Q is even. □

*In fact the number of eigenvalues of power ε^{2r} follows the numbers $N_{K,d-1}$. For example in 2D, one eigenvalue is $\mathcal{O}(\varepsilon^0)$, two eigenvalues are $\mathcal{O}(\varepsilon^2)$, three are $\mathcal{O}(\varepsilon^4)$, ..., and $K+1$ are $\mathcal{O}(\varepsilon^{2K})$.

5.3 Proof of Theorem 4.2

The point set is of type (ii), i.e., it is unisolvent, but the number of points does not coincide with the dimension of a polynomial space. We have $N_{K-1,d} < N < N_{K,d}$ and we can choose N linearly independent polynomials such that (11) holds, for example $\{\underline{x}^{J_K(i)}\}_{i=1}^{N}$. There is no difference between this case and the previous in solving the systems in (15) for $J = 0, \dots, K-1$. However, when we reach the final step, we need to make some further considerations.

P_{-q+K} is a polynomial of degree K. It is either the interpolating polynomial or it is zero in N points. We again assume that $q > 0$ and that the polynomial interpolates zero, but this in itself is not enough to make it identically zero.

We proceed in the following way: First we look at the systems of equations for $J = K$. We can use the fact that $P_{-q+s} \equiv 0$ for $s < K$ to write the systems in block form

$$\begin{pmatrix} A_{p,K-2} & B_p \\ B_p^T & C_p \end{pmatrix} \begin{pmatrix} \underline{\sigma}^i_{p,K}|_{r>0} \\ \underline{\sigma}^i_{p,K}|_{r=0} \end{pmatrix} = \begin{pmatrix} 0 \\ \underline{p}^i_{p,K}|_{s=K} \end{pmatrix}.$$

We then perform block Gaussian elimination on the systems to get

$$(C_p - B_p^T A^{-1}_{p,K-2} B_p)(\underline{\sigma}^i_{p,K}|_{r=0}) = (\underline{p}^i_{p,K}|_{s=K}).$$

This operation is well defined, since $A_{p,K-2}$ is nonsingular, and we also know that the whole system is nonsingular.

Let $\ell_i = J_K(i)$. Then we can express any $\sigma_{-q}^{(\ell_i)}$ with $i > N$ in terms of $\sigma_{-q}^{(\ell_i)}$ with $i \le N$ through relation (12). However, from the systems of equations with $J < K$, we have already determined that $\sigma_{-q}^{(\ell_i)} = 0$ for $i \le N_{K-1,d}$. The total number of unknown moments $\sigma_{-q}^{(\ell_i)}$ left to solve for is $N - N_{K-1,d}$. All of the $(N_{K,d} - N_{K-1,d})$ highest order coefficients in P_{-q+K} can be expressed as combinations of these moments and are hence not independent of each other. That is, the number of degrees of freedom in P_{-q+K} is in fact $N_{K-1,d} + (N - N_{K-1,d}) = N$. Again the assumption that $q > 0$ leads to a contradiction since then $P_{-q+K} = 0$, $\underline{\sigma}_{-q} = 0$, and through (11) $\underline{\lambda}_{-q} = 0$. We must have $q = 0$. The polynomial P_K (of degree K) is uniquely determined by the interpolation conditions. However, the proportions of the highest order coefficients with relation to each other depends on the coefficients a_j for the chosen RBF. The arguments for the modified form of the interpolant when the data is of low degree are the same as in the previous case. □

Example 5.2 *Just to illustrate the method, let us look at the problem in Example 2.1. We have $N = 4$ points and $K = 2$. We can choose the basis $\{1, x, y, x^2\}$. The two systems to solve for $J = K = 2$ are $A_{0,2}\underline{\sigma}_{0,2} = \underline{p}_{0,2}$, and $A_{2,2}\underline{\sigma}_{2,2} = \underline{p}_{2,2}$. Written out, we have*

$$\left(\begin{array}{c|cc} a_0 & a_1 & a_1 \\ \hline a_1 & 6a_2 & 2a_2 \\ a_1 & 2a_2 & 6a_2 \end{array}\right) \left(\begin{array}{c} \sigma_{-q+1}^{(0,0)} \\ \hline \sigma_{-q}^{(2,0)} \\ \sigma_{-q}^{(0,2)}) \end{array}\right) = \left(\begin{array}{c} 0 \\ \hline P_{-q+2}|_{x^2} \\ P_{-q+2}|_{y^2} \end{array}\right) \quad \text{and} \quad 8a_2\sigma_{-q}^{(1,1)} = P_{-q+2}|_{xy}.$$

First we perform Gaussian elimination on the larger system to reduce the number of unknowns. The resulting system is

$$\begin{pmatrix} 6a_2 - \frac{a_1^2}{a_0} & 2a_2 - \frac{a_1^2}{a_0} \\ 2a_2 - \frac{a_1^2}{a_0} & 6a_2 - \frac{a_1^2}{a_0} \end{pmatrix} \begin{pmatrix} \sigma_{-q}^{(2,0)} \\ \sigma_{-q}^{(0,2)}) \end{pmatrix} = \begin{pmatrix} P_{-q+2}|_{x^2} \\ P_{-q+2}|_{y^2} \end{pmatrix}.$$

Then we use (12) to express the higher moments in $\sigma_{-q}^{(2,0)}$*, leading to*

$$\sigma_{-q}^{(1,1)} = -\frac{2}{11}\sigma_{-q}^{(2,0)} \quad \textit{and} \quad \sigma_{-q}^{(0,2)} = -\frac{1}{11}\sigma_{-q}^{(2,0)}.$$

If we let $\sigma_{-q}^{(2,0)} = c_3$ *we can write down the exact form of the interpolating polynomial as*

$$P_2(x,y) = c_0 + c_1 x + c_2 y + \frac{c_3}{11a_0}((64a_0a_2 - 10a_1^2)x^2 - 16a_0a_2xy + (16a_0a_2 - 10a_1^2)y^2).$$

We have exactly 4 unknowns to be determined by the interpolation conditions. As can now be seen, a_0*,* a_1*, and* a_2 *determine which polynomial we will get in the end. If we for example pick IQ,* $a_0a_2 = a_1^2 = 1$ *and the polynomial becomes*

$$P_2(x,y) = c_0 + c_1 x + c_2 y + \frac{c_3}{11}(54x^2 - 16xy + 6y^2),$$

which is in agreement with the result in Example 2.1.

5.4 Proof of Theorem 4.3

When the point set is non-unisolvent (of type (iii)), we have to pick a minimal non-degenerate basis in order to have relation (11). Therefore, the degree of the basis is M instead of K even if $N_{K-1,d} < N \le N_{K,d}$. As an example, for points on the line $x = y$ in two space dimensions, we can choose $\{p_i(\underline{x})\}_{i=1}^N = \{1, x, x^2, x^3, \ldots, x^{N-1}\}$.

The condition that a polynomial P_{-q+s} is zero in N points no longer leads to that the polynomial is zero even if the degree is less than K. Since the problem is non-unisolvent, the polynomial can be zero at the data points, but still contain elements from the nullspace of the degree under consideration. The condition that a polynomial interpolates zero can be expressed as

$$P_{-q+s}(\underline{x}) = n_s(\underline{x}),$$

where $n_s(\underline{x})$ is a nullspace polynomial of degree s. We have not shown yet that P_{-q+s} is of degree s, but when we proceed with solving the sequence of systems (15), we can see that we get the same reduction of degree as in the unisolvent case.

Going back to the example with the line $x = y$, we get nullspace polynomials $n_1(\underline{x}) = \alpha_{11}(x - y)$, $n_2(\underline{x}) = (\alpha_{21} + \alpha_{2x}x + \alpha_{2y}y)(x - y)$, $\ldots$, $n_s(\underline{x}) = p_{s-1}(\underline{x})(x - y)$, where p_{s-1} is an arbitrary polynomial of degree $s - 1$.

As in the unisolvent case, we solve the systems $A_{p,J}\underline{\sigma}_{p,J}^i = \underline{p}_{p,J}^i$ for one J at a time. For a fixed J, we can collect the systems for different p and i into one big system

$$B\underline{\sigma} = \underline{p}. \tag{17}$$

The matrix B is nonsingular, since it is block diagonal with nonsingular blocks $A_{p,J}$. The right hand side contains coefficients from the different nullspace polynomials. We can describe the right hand side as a rectangular matrix C times a vector $\underline{\alpha}$ containing the pertinent nullspace coefficients

$$\underline{p} = C\underline{\alpha}. \tag{18}$$

Each nullspace part in the right hand side corresponds to a relation between the unknown moments. For example, $\alpha_{2x}(x^2 - xy)$ has the counterpart $(\sigma^{(2,0)} - \sigma^{(1,1)}) = 0$. In matrix form, we express this as

$$C^T \underline{\sigma} = 0. \tag{19}$$

Together, equations (17), (18), and (19) define a new system of equations for $\underline{\alpha}$

$$C^T B^{-1} C \underline{\alpha} = 0. \tag{20}$$

The matrix C has full column rank and B is nonsingular. Therefore, the only solution is $\underline{\alpha} = 0$, leading to $\underline{\sigma} = 0$. So far, we have exactly the same result as in the unisolvent case. However, we do not reach the point where assuming that $P_{-q+s} \neq P_K$ leads to a contradiction until $J = M$, since the minimal nondegenerate basis is of order M and we need $\sigma_{-q}^{(\ell)} = 0$ for $|\ell| \leq M$ before $\underline{\lambda}_{-q} = 0$. Hence, we reach the conclusion that $P_{-q+M} = P_K$, $q = M - K$, and the coefficients $\underline{\lambda}$ take the form

$$\underline{\lambda} = \varepsilon^{-2M} \lambda_{-(M-K)} + \varepsilon^{-2M+2} \lambda_{-(M-K)+1} + \cdots.$$

Note that the condition number of the RBF interpolation matrix A is worse for non-unisolvent cases. It can be shown that the largest eigenvalue is $N + \mathcal{O}(\varepsilon^2)$ for any point distribution, whereas the order of the smallest eigenvalue depends on the degree of degeneracy of the point set.

After solving the systems for $J \leq M - 1$, we have lowered the degree of each polynomial P_{-q+s} by M. The first polynomial that still has degree ≥ 0 is $P_{-q+\lceil \frac{M}{2} \rceil} = P_{K-\lfloor \frac{M}{2} \rfloor}$. If M is even it has degree 0, else the degree is 1. Each of the polynomials $P_{K-\lfloor \frac{M}{2} \rfloor}, \ldots, P_{K-1}$ may contain nullspace parts. However, there can be no nullspace part of lower degree than the first nonzero $n_s(\underline{x})$. If we denote this lowest possible nullspace degree by N_0, then the number of polynomials that may be nonzero is reduced to $z = \left\lfloor \frac{M-N_0}{2} \right\rfloor$. The general form of the interpolant is

$$s(\underline{x}, \varepsilon) = \varepsilon^{-2z} P_{K-z}(\underline{x}) + \varepsilon^{-2z+2} P_{K-z+1}(\underline{x}) + \cdots + \varepsilon^{-2} P_{K-1}(\underline{x}) + P_K(\underline{x}) + \mathcal{O}(\varepsilon^2),$$

where the degree of P_{K-j} is $M - 2j$ and the divergent terms only contain polynomial parts that are in the nullspaces. Note that this is a worst case scenario. For example symmetries in the point set can reduce the number of nonzero terms further. However, there are certainly cases where this does not happen and then we get divergence in the interpolant as $\varepsilon \to 0$.

If the data is such that $P_K(\underline{x})$ is of degree $M - Q$, then we get Q extra systems of the type (20). The degree of each divergent term is then reduced by Q and we get $z = \left\lfloor \frac{M-Q-N_0}{2} \right\rfloor$ for the possible number of divergent terms. □

Example 5.3 *We illustrate the non-unisolvent case, by going through Example 2.3. Six points are located on the line* $x = y$. *A minimal non-degenerate basis is* $\{1, x, x^2, x^3, x^4, x^5\}$ *and consequently,* $M = 5$. *Because* $x_k = y_k$ *we know from the start that* $\sigma^{(j_1,j_2)} = \sigma^{(j_1+k, j_2-k)}$. *The nullspaces are*

$$\begin{aligned}
n_1(x,y) &= \alpha_{11}(x-y), \\
n_2(x,y) &= (\alpha_{21} + \alpha_{2x}x + \alpha_{2y}y)(x-y), \\
n_3(x,y) &= (\alpha_{31} + \alpha_{3x}x + \alpha_{3y}y + \alpha_{3x^2}x^2 + \alpha_{3xy}xy + \alpha_{3y^2}y^2)(x-y), \\
n_4(x,y) &= (\alpha_{41} + \alpha_{4x}x + \cdots + \alpha_{4y^3}y^3)(x-y).
\end{aligned}$$

Remember the condition $P_{-q+s}(\underline{x}) = n_s(\underline{x})$*. The task here is to find out which of the coefficients in* n_s *may be nonzero in the final interpolant. Solving the systems for* $J = 0,\ldots,4$*, we get for*

$$\begin{aligned}
J=1: &\quad \alpha_{11}=0,\\
J=2: &\quad \alpha_{2x}=\alpha_{2y}=0,\\
J=3: &\quad \alpha_{3x^2}=\alpha_{3xy}=\alpha_{3y^2}=\alpha_{21}=0,\\
J=4: &\quad \alpha_{4x^3}=\alpha_{4x^2y}=\alpha_{4xy^2}=\alpha_{4y^3}=\alpha_{3x}=\alpha_{3y}=0.
\end{aligned}$$

The parts of the nullspace polynomials that are still undetermined and may appear in the interpolant are $n_3(\underline{x}) = \alpha_{31}(x-y)$ *and* $n_4(\underline{x}) = (\alpha_{41} + \alpha_{4x}x + \alpha_{4y}y + \alpha_{4x^2}x^2 + \alpha_{4xy}xy + \alpha_{4y^2}y^2)(x-y)$*. This is as predicted in the theorem, since* $z = \lfloor \frac{5-1}{2} \rfloor = 2$*. The polynomial that interpolates the data,* $P_K = P_{-q+5} = P_2$*, is of degree five.*

As we are looking at a specific problem, we can go further and see if and how the symmetries may provide some extra benefits. Consider the two systems $A_{1,5}\underline{\sigma}^1_{1,5} = \underline{p}^1_{1,5}$ *and* $A_{1,5}\underline{\sigma}^2_{1,5} = \underline{p}^2_{1,5}$*. The vectors with the unknown moments are*

$$\begin{aligned}
\underline{\sigma}^1_{1,5} &= (\sigma^{(1,0)}_{-q+2},\ \sigma^{(3,0)}_{-q+1},\ \sigma^{(1,2)}_{-q+1},\ \sigma^{(5,0)}_{-q},\ \sigma^{(3,2)}_{-q},\ \sigma^{(1,4)}_{-q})^T,\\
\underline{\sigma}^2_{1,5} &= (\sigma^{(0,1)}_{-q+2},\ \sigma^{(0,3)}_{-q+1},\ \sigma^{(2,1)}_{-q+1},\ \sigma^{(0,5)}_{-q},\ \sigma^{(2,3)}_{-q},\ \sigma^{(4,1)}_{-q})^T,
\end{aligned}$$

but since $x_k = y_k$*, these two vectors are actually identical. The right hand sides are*

$$\begin{aligned}
\underline{p}^1_{1,5} &= (\ \alpha_{31},\quad \alpha_{4x^2},\quad -\alpha_{4xy}+\alpha_{4y^2},\quad P_K|_{x^5},\quad P_K|_{x^3y^2},\quad P_K|_{xy^4})^T,\\
\underline{p}^2_{1,5} &= (-\alpha_{31},\quad -\alpha_{4y^2},\quad -\alpha_{4x^2}+\alpha_{4xy},\quad P_K|_{y^5},\quad P_K|_{x^2y^3},\quad P_K|_{x^4y})^T,
\end{aligned}$$

but if the left hand sides of the two systems are identical, then the right hand sides must also be equal. This immediately gives us

$$\alpha_{31} = 0, \quad \alpha_{4x^2} = -\alpha_{4y^2}, \quad \alpha_{4xy} = 0.$$

Furthermore, we get some symmetry conditions for P_K*. We can proceed further by using the fact that* $\sigma^{(3,0)}_{-q+1} = \sigma^{(1,2)}_{-q+1}$ *and* $\sigma^{(5,0)}_{-q} = \sigma^{(3,2)}_{-q} = \sigma^{(1,4)}_{-q}$*. If we write down the reduced system of equations explicitly we have*

$$-\left(\begin{array}{ccc}
2a_1 & 8a_2 & 24a_3\\
4a_2 & 32a_3 & 160a_4\\
4a_2 & 48a_3 & 288a_4\\
\hline
6a_3 & 80a_4 & 592a_5\\
12a_3 & 224a_4 & 2080a_5\\
6a_3 & 144a_4 & 1360a_5
\end{array}\right)
\left(\begin{array}{c}
\sigma^{(1,0)}_{-q+2}\\
\sigma^{(3,0)}_{-q+1}\\
\sigma^{(5,0)}_{-q}
\end{array}\right)
=
\left(\begin{array}{c}
0\\
\alpha_{4x^2}\\
-\alpha_{4x^2}\\
\hline
P_K|_{x^5}\\
P_K|_{x^3y^2}\\
P_K|_{xy^4}
\end{array}\right).$$

If the 3×3 *upper part of the matrix is non-singular, we can express the moments in* α_{4x^2} *and subsequently the coefficients of order five in* P_K*. This is the case for MQ, IM, and IQ RBFs. However, for the GA and BE RBFs, the* 3×3 *system is singular and the compatibility conditions enforce* $\alpha_{4x^2} = 0$*. In this case, the coefficients of order five can be expressed in one of the moments.*

The same procedure for $J = 6$ yields $\alpha_{4x} = -\alpha_{4y}$. For the MQ, IM and IQ RBFs, the moments and all terms of order four in P_K can be expressed in α_{4x^2} and α_{4x}. For the GA and BE RBF, the nullspace coefficients again become zero and the fourth order terms in P_K can instead be expressed in one of the moments and the terms of order five.

Finally, after going through $J = 7$, 8, and 9, we find that $\alpha_{41} = 0$ for all RBFs and the coefficients in $P_K = P_2$ depend on six parameters, which are uniquely determined by the given data. The interpolant becomes

$$s(\underline{x}, \varepsilon) = \varepsilon^{-2} P_1(\underline{x}) + P_2(\underline{x}) + \mathcal{O}(\varepsilon^2),$$

where $P_1(\underline{x}) = 0$ for GA and BE RBFs, and

$$P_1(\underline{x}) = (\alpha_{4x}(x-y) + \alpha_{4x^2}(x^2 - y^2))(x-y) = (\alpha_{4x} + \alpha_{4x^2}(x+y))(x-y)^2,$$

for MQ, IM and IQ RBFs. The coefficients in P_1 and P_2 depend on the chosen RBF. Going back to the results in Example 2.3, we find that the form of P_1 is in exact agreement.

So why is it that the GA interpolant does not diverge? This may seem like a coincidence, but we have seen the same behavior in every example we have studied and in our numerical experiments as well. In [21] we conjecture that the GA RBF never diverges and supply proofs for some special cases. Why the BE interpolant does not diverge is a slightly different story, which will be commented upon in the following section.

6 Explanations and discussion

We have already looked at Examples 2.1 and 2.3 in connection with the proofs. Example 2.4 is the unisolvent case with $N = N_{2,2} = 6$. Except for the BE RBF, the results are as predicted by Theorem 4.1. For further discussion of the BE RBF, see subsection 6.3.

6.1 Example 2.2

The point set is non-unisolvent and the points are located on the parabola $y = x^2$. A minimal non-degenerate basis is $\{1, x, y, xy, y^2, x^3\}$, meaning that $M = 3$. The lowest degree nullspace is $n_2(\underline{x}) = \alpha_1(y - x^2)$ and $z = \lfloor \frac{M-N_0}{2} \rfloor = 0$. There can be no divergent terms, but the limit does depend on the RBF.

If we use more points on a parabola, we do get divergence. The first divergent case is for $N = 8$ points with a term of order ε^{-2} [21]. In this case $M = 4$ and $N_0 = 2$ leading to $z = 1$. Accordingly, the worst case actually occurs here.

6.2 Example 2.5

Somewhat unexpectedly, we get the same result for all RBFs in this case, even though the points are on circle and we do have a nullspace. The equation for the circle is $(x - \frac{1}{2})^2 + (y - \frac{1}{2})^2 = \frac{1}{4}$ or $y^2 = -\frac{1}{4} + x + y - x^2$. A minimal non-degenerate basis is $\{1, x, y, x^2, xy, x^3\}$ and the first nullspace polynomial is

$$n_2(x, y) = \alpha_1(x^2 + y^2 - x - y + \tfrac{1}{4}).$$

Again $M = 3$ and $N_0 = 2$ and there can be no divergent terms. From the equations for $J = 0, \dots, 2$ we get $\sigma_{-q}^{(j)} = 0,\ |j| \le 2$ and $\sigma_{-q+1}^{(j)} = 0,\ |j| = 0$. When we look at the equations for $J \ge 3$, we can use relation (12) to reduce the number of unknown moments. If we for example take $A_{1,3}\underline{\sigma}_{1,3}^1 = \underline{p}_{1,3}^1$ and use $\sigma_{-q}^{(1,2)} = -\sigma_{-q}^{(3,0)}$, the system

$$-\begin{pmatrix} 2a_1 & 4a_2 & 4a_2 \\ 4a_1 & 20a_3 & 12a_3 \\ 4a_2 & 12a_3 & 36a_3 \end{pmatrix}\begin{pmatrix} \sigma_{-q+1}^{(1,0)} \\ \sigma_{-q}^{(3,0)} \\ \sigma_{-q}^{(1,2)} \end{pmatrix} = \begin{pmatrix} 0 \\ P_{-q+3}|_{x^3} \\ P_{-q+3}|_{xy^2} \end{pmatrix}$$

is reduced to

$$\begin{pmatrix} -8a_3 \\ 24a_3 \end{pmatrix}\begin{pmatrix} \sigma_{-q}^{(3,0)} \end{pmatrix} = \begin{pmatrix} P_{-q+3}|_{x^3} \\ P_{-q+3}|_{xy^2} \end{pmatrix}.$$

The relative size of the two coefficients in $P_{-q+3} = P_K$ does not depend on the RBF because of the way the moments cancelled each other out in the first (homogeneous) equation. The fact that the points are on a circle lead to the same type of relation between the moments and subsequent cancellations in all systems where the coefficients of the limit interpolant are present and the final form of the polynomial is

$$\begin{aligned} P_{-q+3}(x, y) &= s_1(8x^3 - 24xy^2) + (4s_2 + 12s_1)(x^2 - y^2) + (8s_3 - 24s_1)xy \\ &+ s_4x + s_5y + s_6. \end{aligned}$$

The six unknown parameters in the polynomial are the same for all RBFs and are uniquely determined by the given data. The result is $s_1 = s_6 = \frac{1}{6}$, $s_2 = s_4 = s_5 = -\frac{4}{6}$, and $s_3 = 1$, leading to the polynomial in Example 2.5.

In all the experiments we have done, we have never managed to get divergence, or even different limits for different RBFs, for points on any circle. We believe this is exactly because of the cancellation property of the moments. There may be divergence for larger number of points, but our guess is that the result holds independently of N.

6.3 The BE RBF and other special functions

In Example 2.4 all RBFs except the BE RBF have the same limit, which is the unique interpolating polynomial of degree two. The reason for the deviant behavior is that the expansion coefficients of the BE RBF do not fulfill the non-singularity condition (III).

Conjecture 6.1 *All matrices $A_{p,K}$ with $K > 1$ are singular for the expansion coefficients of the BE RBF.*

There is (at least) one function with this property in all even dimensions and some odd dimensions. Table 4 shows some of the functions. Some properties that these special functions have in common are

- They seem to fail the conditions $\det(A_{p,K}) \ne 0$ for $K > 1$.
- They are the lowest radial eigenmodes that are bounded at the origin of the Laplacian in d dimensions. The equation they solve is

$$\phi'' + \frac{(d-1)}{r}\phi' + \phi = 0.$$

Table 4: Functions with special behavior in d dimensions.

d	Function
1	$\cos(r)$
2	$J_0(r)$
3	$\text{sinc}(r)$
4	$J_1(r)/r$
5	No bounded solution.
6	$J_2(r)/r^2$
7	No bounded solution.
8	$J_3(r)/r^3$

- They have compact support in the Fourier domain.

Using these functions as RBFs in the dimension where they are special does not seem to be a good idea, at least not for smooth data, since the results are not very accurate. However, the special functions do seem less prone to divergence for non-unisolvent point sets. They can be used in a lower dimension (except for $\cos(r)$) and give results similar to other RBFs. However, at least in dimensions higher than d these functions may lead to singular RBF matrices, which is not a very desirable property.

7 The principle behind errors and optimal shape parameter values for smooth functions

A number of authors have performed theoretical studies of the dependence on h of the errors in radial basis function interpolants, where

$$h = \sup_{\underline{x}\in\Omega} \min_{1\leq k\leq N} \|\underline{x} - \underline{x}_k\|$$

measures the point density in Ω, the domain under consideration. For smooth data functions and smooth RBFs the convergence is spectral in h [25, 19, 20, 17]. The dependence on the shape parameter ε has been less studied. Madych [19] gives an error bound proportional to $\lambda^{1/(h\varepsilon)}$ for ε in the range $1/a \leq \varepsilon \leq 1$, where a is the diameter of Ω and $0 < \lambda < 1$. Cheng *et al.* [26] found through numerical experiments that the error behaves as $\lambda^{1/(h\sqrt{\varepsilon})}$. Several other authors have noted that the quality of the solution depends strongly on the shape parameter and that there is an optimal shape parameter value, which depends on the function to be interpolated, the node points, the RBF, and the machine precision, see e.g. [27, 28, 29]. Different methods to locate the optimal shape parameter are also proposed in these articles.

However, in many cases, it is not possible to compute the solution at the best ε-value directly in finite precision arithmetic due to the severe ill-conditioning of the RBF interpolation matrix. This is illustrated by the uncertainty principle of Wu and Schaback [30], which says that the attainable error and the condition number of the RBF interpolation matrix cannot both be small at the same time. The condition number grows both with decreasing h and decreasing ε.

A method which circumvents the ill-conditioning and makes it possible to solve the RBF interpolation problem for any value of the shape parameter ε for point sets of moderate size was recently developed [16]. When we started to do experiments with the method and computing solutions for very small values of the shape parameter, we found that for smooth functions, the error often has a minimum for some small non-zero value of ε. This behavior is not limited to the interpolation problem, but shows also for example when solving PDEs using RBF collocation methods [11]. Examples of typical error curves can be seen in Figure 1.

This is not an artifact of the solution method. It is the actual behavior of the error. In the following subsections, we look at which parameters determine the optimal shape parameter values (and the overall ε-dependence in the error), using the techniques from the proofs in Section 5. We are able to give a reasonable description of the behavior for small ε, a region which has until recently been very little explored. First we discuss the error in general. Then we consider the one-dimensional and two-dimensional cases, and finally we take a quick look at the special case of polynomial data.

7.1 General properties

We consider problems with unisolvent point sets, where we want to find an interpolant to a smooth multivariate function $f(\underline{x})$. In order to express the error in a useful way, we use Taylor expansions of both the function and the RBF interpolant around $\underline{x} = \underline{0}$. For the function, using multi-index notation, we get

$$f(\underline{x}) = f(\underline{0}) + \frac{\partial f}{\partial x_1}(\underline{0})x_1 + \frac{\partial f}{\partial x_2}(\underline{0})x_2 + \ldots = \sum_{j \in J_\infty} f_j x^j, \quad \text{where } f_j = \frac{f^{(j)}(\underline{0})}{j!}. \tag{21}$$

For the interpolant, we use the expansion from Theorem 4.1,

$$s(\underline{x}, \varepsilon) = P_K(\underline{x}) + \varepsilon^2 P_{K+1}(\underline{x}) + \varepsilon^4 P_{K+2}(\underline{x}) + \cdots \equiv \sum_{j \in J_\infty} s_j(\varepsilon)\underline{x}^j, \tag{22}$$

where, using that the degree of P_{K+m} is $K + 2m$,

$$s_j(\varepsilon) = \sum_{m=\max(0,\lceil \frac{|j|-K}{2} \rceil)}^{\infty} \varepsilon^{2m} P_{K+m}|_{\underline{x}^j}. \tag{23}$$

The polynomial $P_K(\underline{x})$ is the unique interpolating polynomial of degree K for the data given at $N = N_{K,d}$ node points. If we let $P_K(\underline{x}) = \sum_{j \in J_K} p_j \underline{x}^j$, the following holds for $s_j(\varepsilon)$:

$$s_j(\varepsilon) = \begin{cases} p_j + \mathcal{O}(\varepsilon^2), & |j| \le K, \\ \mathcal{O}(\varepsilon^{2r}), \quad r = \left\lceil \frac{|j|-K}{2} \right\rceil, & |j| > K. \end{cases} \tag{24}$$

The error in the interpolant can be expressed as an infinite expansion in powers of $\underline{x}$ by combining (21) and (22),

$$e(\underline{x}, \varepsilon) = s(\underline{x}, \varepsilon) - f(\underline{x}) = \sum_{j \in J_\infty} [s_j(\varepsilon) - f_j]\, \underline{x}^j = \sum_{j \in J_\infty} e_j(\varepsilon)\underline{x}^j. \tag{25}$$

If we study the error expansion, there are a few things we can say in general

- The error is zero for all $\underline{x}$ if and only if $s_j(\varepsilon) = f_j$ for all j.This happens exactly if
  i) The function $f(\underline{x}) \equiv \sum_{k=1}^{N} \lambda_k \phi(\varepsilon \|\underline{x} - \underline{x}_k\|)$ for some λ_k and ε.
  ii) The function $f(\underline{x})$ is a polynomial of degree $J \leq K$. Then $f_j = p_j,\ |j| \leq K$ and the error is zero for $\varepsilon = 0$.
- If none of the situations above apply, each term in the error expansion has an optimal value of ε, for which it is minimized. These ε may all be different, but there will still be one or more global minima for which we get the overall best solution.
- If $f(\underline{x})$ is smooth with a convergent Taylor series in the domain of interest and if ε is small enough for the expansion of $s(\underline{x}, \varepsilon)$ to converge, then the error expansion is convergent and truncation of the sum gives an approximation of the error.
- The error is (always) exactly zero at the N collocation points, because of the interpolation conditions.

Remark: The notion of ε being small enough has to do with the convergence radius R of the expansion (8). We need to have $\varepsilon^2 r_k^2 < R$, for all r_k. The radius is $R = 1$ for MQ, IM, and IQ, whereas for GA we have an infinite radius of convergence.

Under the assumption that the f_j decay rapidly and that ε is small, we can write down a series of approximate error expansions $\tilde{e}_r(\underline{x}, \varepsilon)$, where all terms of order up to ε^{2r} from the interpolant and the corresponding f_j are included. Let $P_{K+1} = \sum_{j \in J_{K+2}} q_j \underline{x}^j$ and let $P_{K+2} = \sum_{j \in J_{K+4}} t_j \underline{x}^j$. Then the approximations of order ε^2 and ε^4 are

$$\tilde{e}_1(\underline{x}, \varepsilon) = \sum_{j \in J_K} \left[p_j - f_j + \varepsilon^2 q_j\right] \underline{x}^j + \sum_{j \in J_{K+2} \setminus J_K} \left[\varepsilon^2 q_j - f_j\right] \underline{x}^j, \tag{26}$$

$$\begin{aligned} \tilde{e}_2(\underline{x}, \varepsilon) \quad &= \sum_{j \in J_K} \left[p_j - f_j + \varepsilon^2 q_j + \varepsilon^4 t_j\right] \underline{x}^j + \sum_{j \in J_{K+2} \setminus J_K} \left[\varepsilon^2 q_j + \varepsilon^4 t_j - f_j\right] \underline{x}^j \\ &+ \sum_{j \in J_{K+4} \setminus J_{K+2}} \left[\varepsilon^4 t_j - f_j\right] \underline{x}^j. \end{aligned} \tag{27}$$

In the two following subsections, these approximations are tested against the actual computed errors to see if they are accurate enough to describe the true behavior of the error.

7.2 The one dimensional case

For ease of discussion, consider a problem in one dimension. The exact error is exactly zero at the node points. The approximate errors $\tilde{e}_r$ are not exactly zero at the node points, but if the discarded f_j are small enough, the difference is negligible. Assuming this, the approximate error (26) is a polynomial of degree $K + 2 = N + 1$, which is zero at the N node points and can be written

$$\tilde{e}_1(x, \varepsilon) \quad \approx \quad (ax + b) \prod_{k=1}^{N} (x - x_k) \tag{28}$$

$$= \quad ax^{K+2} + (b - a\sum_{k=1}^{N} x_k)x^{K+1} + \ldots + b(-1)^N \sum_{k=1}^{N} x_k.$$

By identifying the right hand side in (28) with expansion (26), we find that

$$a(\varepsilon) \quad = \quad \varepsilon^2 q_{K+2} - f_{K+2}, \tag{29}$$

$$b(\varepsilon) \quad = \quad \varepsilon^2 q_{K+1} - f_{K+1} + a(\varepsilon)\sum_{k=1}^{N} x_k. \tag{30}$$

The same approach for expansion (27) yields

$$\tilde{e}_2(x,\varepsilon) \quad \approx \quad (ax^3 + bx^2 + cx + d)\prod_{k=1}^{N}(x - x_k), \quad \text{where} \tag{31}$$

$$a(\varepsilon) \quad = \quad \varepsilon^4 t_{K+4} - f_{K+4}, \tag{32}$$

$$b(\varepsilon) \quad = \quad \varepsilon^4 t_{K+3} - f_{K+3} + a(\varepsilon)\sum_{k=1}^{N} x_k, \tag{33}$$

$$c(\varepsilon) \quad = \quad \varepsilon^4 t_{K+2} + \varepsilon^2 q_{K+2} - f_{K+2} + b(\varepsilon)\sum_{k=1}^{N} x_k - \frac{a(\varepsilon)}{2}\sum_{j\neq k} x_j x_k \tag{34}$$

$$\begin{aligned} d(\varepsilon) \quad &= \quad \varepsilon^4 t_{K+1} + \varepsilon^2 q_{K+1} - f_{K+1} \\ &+ \quad c(\varepsilon)\sum_{k=1}^{N} x_k - \frac{b(\varepsilon)}{2}\sum_{j\neq k} x_j x_k + \frac{a(\varepsilon)}{6}\sum_{i\neq j\neq k,\ i\neq k} x_i x_j x_k \end{aligned} \tag{35}$$

From equations (28) and (31) it is clear that the error approximations have two almost independent parts. The first part is mainly determined by the choice of ε and the function we are trying to approximate. The second part (the product of zeros) only depends on the collocation points. If the points are uniformly distributed in the interval $[a,b]$ and $h = (b-a)/(N-1)$ is the distance between adjacent points, then we have the estimate

$$\max_{x\in[a,b]} \prod_{k=1}^{N}(x - x_k) < (N-1)!\, h^N = \frac{(N-1)!}{(N-1)^N} \approx \sqrt{2\pi}\, h^{1/2}\, e^{-1/h},$$

where Stirling's formula for the factorial was used for the final approximation. This part alone corresponds to a spectral rate of convergence. By choosing ε such that the coefficients a and b, or a, b, c , and d are minimized, the error can be reduced even further. The more rapid the decay of f_j is, the smaller the optimal value of ε becomes, as will be illustrated in more detail in an example. Note that if the data is polynomial of degree $\leq K$, all f_j with $|j| > K$ are zero, and the optimal value of the shape parameter is $\varepsilon = 0$, giving the exact solution. Figures 1 and 2 show the exact and approximate errors in maximum norm for the two functions

$$\begin{aligned} f_1(x) \quad &= \quad \frac{65}{65 + (x - 1/5)^2}, \\ f_2(x) \quad &= \quad \sin(x). \end{aligned}$$

The data points are unevenly distributed throughout the interval $[-1, 1]$ and the error,

$$E(\varepsilon) = \max_{x \in [-1,1]} e(x, \varepsilon),$$

is evaluated using a fine uniform point distribution. The errors given by the approximations $\tilde{e}_r$ agree very well with the exact errors. Accordingly, it is reasonable to use the approximations to explain the error curves. The order of the approximation needs to be increased with N in order to get good agreement all the way up to the radius of convergence. This is not unexpected, since for larger N, the error is smaller, and smaller terms become relatively more significant. With the length of the interval being $a = 2$, we can not expect the approximations to converge for $\varepsilon > 1/2$ in the case of MQ RBFs. For GA RBFs, even if the radius of convergence is infinite, the number of terms that are needed for large values of ε grows fast and we only show results for $\varepsilon \leq 1$.

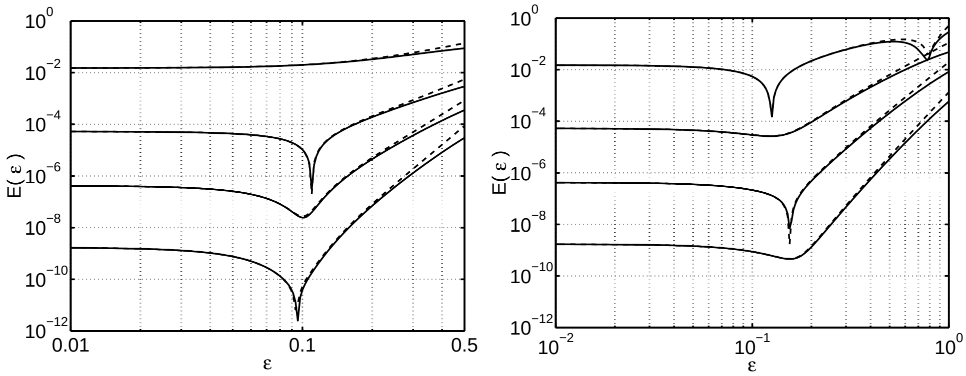


Figure 1: The error in the computed solution (solid lines) for $f_1(x)$ for $N = 2, 4, 6$ and 8 points and the approximation $\tilde{e}_{N/2}$ of the error (except for $N = 2$ to the right, where $\tilde{e}_{N/2+1}$ is used) (dashed lines). The left part of the figure shows the result for MQ RBFs and the right part corresponds to GA RBFs.

The ε-dependence in the approximate error curves comes from the coefficients a, b, ..., but is somewhat influenced by the placement of the node points. For most of the error curves there are clear optima. In order to see exactly where and how these optima arise, we go through an example in detail.

Example 7.1 *Consider a one-dimensional problem with $N = 4$ distinct points x_j, $j = 1, \ldots, 4$. The interpolating polynomial $P_K = P_3$ has degree 3. We can use $\{1, x, x^2, x^3\}$ as a basis, meaning that any moment $\sigma^{(j)}$ with $j > 3$ can be expressed in moments with $j \leq 3$ using relation (12). As a first step, we compute the polynomials P_4 and P_5 expressed in the coefficients of P_3. In order to do this, we use the systems (15), but add extra equations for the higher polynomial coefficients. The systems for $J = 3$ and $J = 4$ are*

$$-\begin{pmatrix} 2a_1 & 4a_2 \\ 4a_2 & 20a_3 \\ 6a_3 & 56a_4 \\ 8a_4 & 120a_5 \end{pmatrix} \begin{pmatrix} \sigma_1^{(1)} \\ \sigma_0^{(3)} \end{pmatrix} = \begin{pmatrix} 0 \\ p_3 \\ q_5 \\ t_7 \end{pmatrix},$$

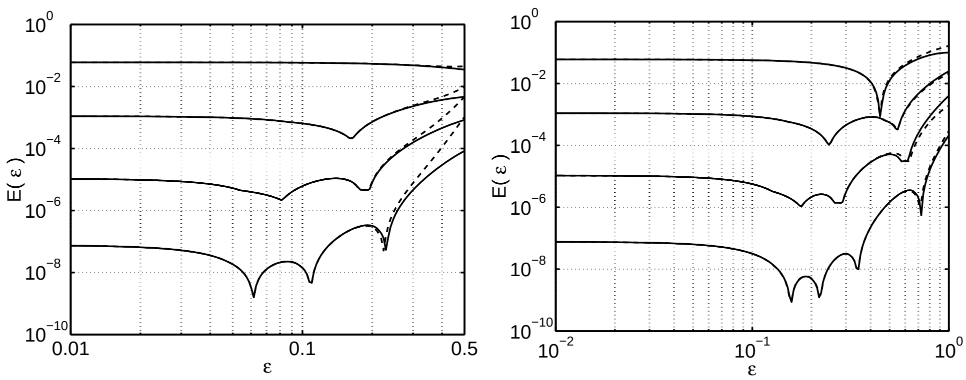


Figure 2: The error in the computed solution (solid lines) for $f_2(x)$ for $N = 2, 4, 6$ and 8 points and the approximation $\tilde{e}_{N/2+1}$ of the error (except for $N = 8$ to the right, where $\tilde{e}_{N/2+2}$ is used) (dashed lines). The left part of the figure shows the result for MQ RBFs and the right part corresponds to GA RBFs.

$$\begin{pmatrix} a_0 & a_1 & a_2 \\ a_1 & 6a_2 & 15a_3 \\ a_2 & 15a_3 & 70a_4 \\ a_3 & 28a_4 & 210a_5 \end{pmatrix} \begin{pmatrix} \sigma_2^{(0)} \\ \sigma_1^{(2)} \\ \sigma_0^{(4)} \end{pmatrix} = \begin{pmatrix} 0 \\ p_2 \\ q_4 \\ t_6 \end{pmatrix}.$$

Together with the requirement that $P_4(x_j) = 0$, $j = 1, \ldots, 4$, we can determine all of the coefficients q_j, $j = 0, \ldots, 5$ using these equations. Similarly, $P_5(x_j) = 0$ together with the systems for $J = 5$ and $J = 6$ below determines $P_5(x)$ completely.

$$-\begin{pmatrix} 2a_1 & 4a_2 & 6a_3 \\ 4a_2 & 20a_3 & 56a_4 \\ 6a_3 & 56a_4 & 252a_5 \end{pmatrix} \begin{pmatrix} \sigma_2^{(1)} \\ \sigma_1^{(3)} \\ \sigma_0^{(5)} \end{pmatrix} = \begin{pmatrix} p_1 \\ q_3 \\ t_5 \end{pmatrix}$$

$$\begin{pmatrix} a_0 & a_1 & a_2 & a_3 \\ a_1 & 6a_2 & 15a_3 & 28a_4 \\ a_2 & 15a_3 & 70a_4 & 210a_5 \end{pmatrix} \begin{pmatrix} \sigma_3^{(0)} \\ \sigma_2^{(2)} \\ \sigma_1^{(4)} \\ \sigma_0^{(6)} \end{pmatrix} = \begin{pmatrix} p_0 \\ q_2 \\ t_4 \end{pmatrix}$$

If we choose MQ as the RBF and $\{-1, -\frac{1}{2}, \frac{1}{3}, 1\}$ as our data points, the resulting polynomials are

$$P_4(x) = \frac{p_3}{144}(-288x^5 - 42x^4 + 337x^3 + 41x^2 - 49x + 1) + \frac{p_2}{6}(-6x^4 - x^3 + 7x^2 + x - 1).$$

$$\begin{aligned} P_5(x) = {} & \frac{p_3}{20736}\left(64800x^7 + 15984x^6 - 28944x^5 - 16782x^4 \right. \\ & \qquad \left. -44749x^3 + 2059x^2 + 8893x - 1261\right) \\ & + \frac{p_2}{1728}\left(1944x^6 + 576x^5 + 1596x^4 + 19x^3 - 4177x^2 - 595x + 637\right) \\ & + \frac{p_1}{144}\left(-90x^5 - 21x^4 + 104x^3 + 22x^2 - 14x - 1\right) + \frac{p_0}{16}\left(6x^4 + x^3 - 7x^2 - x + 1\right). \end{aligned}$$

Substituting the coefficients of P_4 and P_5 into the approximation (31) for $e_2(x,\varepsilon)$, we get the following expressions for the coefficients in the error polynomial

$$
\begin{aligned}
a(\varepsilon) &= \frac{25}{8}p_3\varepsilon^4 - f_7,\\
b(\varepsilon) &= \left(\frac{1}{4}p_3 + \frac{9}{8}p_2\right)\varepsilon^4 - f_6 + \frac{1}{6}f_7,\\
c(\varepsilon) &= \left(\frac{53}{24}p_3 + \frac{7}{48}p_2 - \frac{5}{8}p_1\right)\varepsilon^4 - 2p_3\varepsilon^2 - f_5 + \frac{1}{6}f_6 - \frac{43}{36}f_7,\\
d(\varepsilon) &= \left(-\frac{1261}{3456}p_3 + \frac{637}{288}p_2 - \frac{1}{24}p_1 + \frac{3}{8}p_0\right)\varepsilon^4 + \left(\frac{1}{24}p_3 - p_2\right)\varepsilon^2\\
&- f_4 + \frac{1}{6}f_5 - \frac{43}{36}f_6 + \frac{49}{216}f_7.
\end{aligned}
$$

If the coefficients in the Taylor expansion of the function $f(x)$ decay rapidly, the function is well approximated by the interpolating polynomial and $p_j \approx f_j$. Therefore, it is reasonable to assume that $d(\varepsilon)$ will be the dominant coefficient in such a case, since it depends on the lowest order p_j and f_j. This is true for the function $f_1(x)$, where furthermore f_{2j} is significantly larger than f_{2j+1}. The coefficients a, b, c, and d are shown in the left part of Figure 3. As expected, the largest coefficient is $d(\varepsilon)$, which is approximately given by

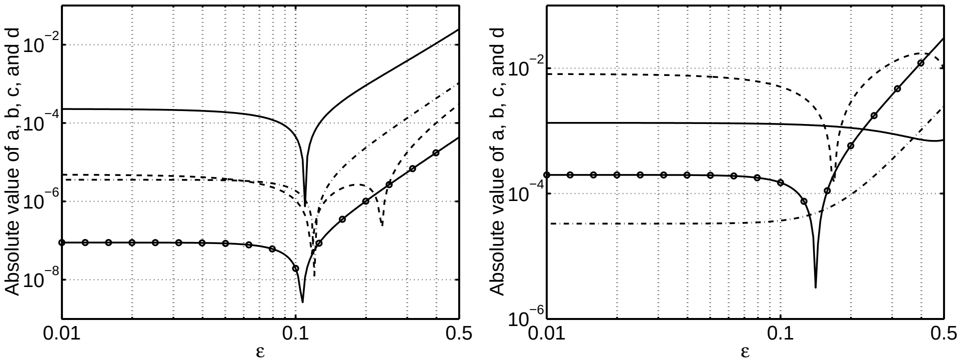


Figure 3: The coefficients $a(\varepsilon)$ (with circles), $b(\varepsilon)$ (dash-dot line), $c(\varepsilon)$ (dashed line), and $d(\varepsilon)$ (solid line) in the error approximation (31) for the functions $f_1(x)$ (left) and $f_2(x)$ (right) using MQ RBFs.

$$d(\varepsilon) \approx \frac{3}{8}p_0\varepsilon^4 - p_2\varepsilon^2 - f_4,$$

leading to the optimal ε-value

$$(\varepsilon^*)^2 = \frac{8}{6}\frac{p_2}{p_0} + \sqrt{\left(\frac{8}{6}\frac{p_2}{p_0}\right)^2 + \frac{8}{3}\frac{f_4}{p_0}} \approx 0.012 \quad \Rightarrow \quad \varepsilon^* \approx 0.11.$$

A comparison with the computed errors in Figure 1 shows that this is exactly the optimal ε *for this problem. (The point set here is the same as for* $N = 4$ *in the figure.) If we use the simpler approximation (28) with terms only up to* ε^2*, the coefficients are*

$$\begin{aligned} a(\varepsilon) &= -2p_3\varepsilon^2 - f_5, \\ b(\varepsilon) &= \left(\frac{1}{24}p_3 - p_2\right)\varepsilon^2 - f_4 + \frac{1}{6}f_5. \end{aligned}$$

Here, $b(\varepsilon)$ *is the largest coefficient, leading to*

$$(\varepsilon^*)^2 \approx -\frac{f_4}{p_2} \approx 0.0156 \quad \Rightarrow \quad \varepsilon^* \approx 0.12,$$

which is also a good approximation of the optimal value for the shape parameter.

The Taylor expansion of the function f_2 *decays more slowly initially, and all even Taylor coefficients are zero. The coefficients a, b, c, and d from the approximation (31) are shown in the right part of Figure 3. For this function,* $c(\varepsilon)$ *is the largest coefficient, since* $p_0 \approx 0$*. The optimal values of the shape parameter given by the largest coefficient in* $\tilde{e}_2(x,\varepsilon)$ *and* $\tilde{e}_1(x,\varepsilon)$ *respectively become*

$$(\varepsilon^*)^2 \approx \frac{24p_3 \pm 2\sqrt{144p_3^2 + 6f_5(53p_3 - 15p_1)}}{53p_3 - 15p_1} \approx 0.0292 \text{ (and } 0.294) \quad \Rightarrow \quad \varepsilon^* \approx 0.17,$$

$$(\varepsilon^*)^2 \approx -\frac{1}{2}\frac{f_5}{p_3} \approx 0.0265 \quad \Rightarrow \quad \varepsilon^* \approx 0.16.$$

Again, the approximate values are very close to the computed optimal value, which is about 0.16 as can be seen in Figure 2. If we instead use the expansion coefficients for the GA RBF in all of the computations above for the function $f_2(x)$*, we get a different optimum. The simpler approximation yields*

$$(\varepsilon^*)^2 \approx -\frac{f_5}{p_3} \approx 0.0531 \quad \Rightarrow \quad \varepsilon^* \approx 0.23.$$

Comparing with the right part of Figure 2, this result is also very close to the computed optimal value, which is approximately 0.25.

We can not give an exact formula for the optimal ε for an arbitrary problem. The optima depend on the solution function, the RBF, the size of the point set, and to a lesser degree, the distribution of the points. However, we can give some general properties of the ε-dependence of the error for RBF interpolation of smooth functions (in one dimension)

- The optimal ε-value depends on the RBF. In our numerical experiments, we have found that the optima for MQ, IM, and IQ RBFs are similar, whereas the GA RBF typically has a larger optimal value.
- The ε-dependence of the error is well described by the coefficients in the error approximations $\tilde{e}_r$. These coefficients are polynomials of order r in ε^2. Therefore, an error curve which is well approximated by $\tilde{e}_r$ may have r local minima. Since r grows with N, the number of local minima typically grows with N as for the function $f_2(x)$ in Figure 2.

- The optimal ε-value depends on the decay rate of the Taylor expansion of the function under consideration. A function with a faster decay has a smaller optimal value. This can be seen in the following way: A function with a rapidly decaying Taylor series is close to its interpolating polynomial. Only a small correction to the limit interpolant at $\varepsilon = 0$ is needed.

- Starting at a large ε-value, the error decreases rapidly as ε becomes smaller. The rate of decrease is higher for larger N. From $\varepsilon = 1$ down to just before the optimal value, we can confirm the result of [26] that the error curve behaves as $C \exp(c/\sqrt{\varepsilon})$, where C and $c < 0$ may depend on N, but not ε. After the optimal ε-value, the error increases a little bit and levels out at the polynomial interpolation error (since the $\varepsilon = 0$ limit gives the interpolating polynomial).

Note that the decay rate is not the only property of the Taylor expansion that has an influence on the error. In the example above, for a function where f_j and f_{j+2} have the same sign, the optimal ε on the real axis is $\varepsilon = 0$ (which does not give the exact solution). In these cases, the true optimum is actually on the imaginary axis, $\varepsilon = i\alpha$. Normally, only real values of the shape parameter are used in RBF interpolation, since non-singularity of the coefficient matrix A in (2) cannot be guaranteed otherwise. However, with the Contour–Padé algorithm [16] we can safely compute for whole regions in the complex ε-plane and have actually observed this.

7.3 The two-dimensional case

In two space dimensions (or more) we do not get the simple factorization of the error approximations into two parts that we had in one dimension. The error is still zero at all node points, but there is no simple way to express this in general. However, if we consider the approximations (26) and (27), we can instead see it in the following way: All coefficients in the polynomial with $|j| > K$ depend on ε and the function that is being approximated. By an appropriate choice of the shape parameter, these can be made as small as possible. The other coefficients with $|j| \le K$ are determined by the condition $e(\underline{x}_k, \varepsilon) = 0,\ k = 1, \ldots, N$.

In the same way as for the one-dimensional case, we can go through an example to see exactly how the optimal ε-value depends on the highest order coefficients in $\tilde{e}_1(\underline{x}, \varepsilon)$ and what the error curves look like.

Example 7.2 *Consider an interpolation problem in two space dimensions with $N = 6$ points. We assume that the point set is chosen in such a way that the problem is unisolvent. Then the limiting interpolant has degree $K = 2$. A suitable basis is $\{1, x, y, x^2, xy, y^2\}$. Using the systems (15) for $J = 2$ and $J = 3$ together with relation (12), we can determine all the highest coefficients in P_3 in terms of the limit interpolant P_2. If we use MQ RBFs and let the data points be $\underline{x}_1 = (1/10, 4/5)$, $\underline{x}_2 = (1/5, 1/5)$, $\underline{x}_3 = (3/10, 1)$, $\underline{x}_4 = (3/5, 1/2)$, $\underline{x}_5 = (4/5, 3/5)$, and $\underline{x}_6 = (1, 1)$, the resulting polynomial is*

$$
\begin{aligned}
P_3(x,y) = {} & p_{2,0}\left(-\tfrac{7}{6}x^4 - \tfrac{5}{6}x^2y^2 + \tfrac{1}{3}y^4 + \tfrac{14731}{8625}x^3 + \tfrac{1271}{1150}x^2y + \tfrac{3232}{8625}xy^2 - \tfrac{2899}{2875}y^3\right) \\
& + p_{1,1}\left(-\tfrac{3}{2}x^3y - \tfrac{3}{2}xy^3 + \tfrac{3492}{2875}x^3 + \tfrac{4031}{1150}x^2y + \tfrac{46821}{11500}xy^2 + \tfrac{12209}{11500}y^3\right) \\
& + p_{0,2}\left(\tfrac{1}{2}x^4 - \tfrac{5}{6}x^2y^2 - \tfrac{7}{6}y^4 - \tfrac{7097}{8625}x^3 - \tfrac{451}{575}x^2y - \tfrac{6943}{17250}xy^2 + \tfrac{5563}{2875}y^3\right) \\
& + p_{1,0}\left(-\tfrac{1}{2}x^3 - \tfrac{1}{2}xy^2\right) + p_{0,1}\left(-\tfrac{1}{2}x^2y - \tfrac{1}{2}y^3\right) \\
& + c_1x^2 + c_2xy + c_3y^2 + c_4x + c_5y + c_6.
\end{aligned}
$$

The six remaining coefficients can be determined from $P_3(x_k, y_k) = 0,\ k = 1, \dots, N$. We can now write down the coefficients $e_j(\varepsilon)$ for all terms with $|j| = K+1$ and $|j| = K+2$ in the approximate error $\tilde{e}_1(\underline{x}, \varepsilon)$,

$$\begin{aligned}
e_{4,0} &= \left(-\tfrac{7}{6}p_{2,0} + \tfrac{1}{3}p_{0,2} \right)\varepsilon^2 - f_{4,0},\\
e_{0,4} &= \left(\tfrac{1}{3}p_{2,0} - \tfrac{7}{6}p_{0,2} \right)\varepsilon^2 - f_{0,4},\\
e_{2,2} &= \left(-\tfrac{5}{6}p_{2,0} - \tfrac{5}{6}p_{0,2} \right)\varepsilon^2 - f_{2,2},\\
e_{3,1} &= \left(- \tfrac{3}{2}p_{1,1} \right)\varepsilon^2 - f_{3,1},\\
e_{1,3} &= \left(- \tfrac{3}{2}p_{1,1} \right)\varepsilon^2 - f_{1,3},\\
e_{3,0} &= \left(\tfrac{14731}{8625}p_{2,0} - \tfrac{7097}{8625}p_{0,2} + \tfrac{3492}{2875}p_{1,1} - \tfrac{1}{2}p_{1,0} \right)\varepsilon^2 - f_{3,0},\\
e_{0,3} &= \left(-\tfrac{2899}{2875}p_{2,0} + \tfrac{5563}{2875}p_{0,2} + \tfrac{12209}{11500}p_{1,1} - \tfrac{1}{2}p_{0,1} \right)\varepsilon^2 - f_{0,3},\\
e_{2,1} &= \left(\tfrac{1271}{1150}p_{2,0} - \tfrac{451}{575}p_{0,2} + \tfrac{4031}{1150}p_{1,1} - \tfrac{1}{2}p_{0,1} \right)\varepsilon^2 - f_{2,1},\\
e_{1,2} &= \left(\tfrac{3232}{8625}p_{2,0} - \tfrac{6943}{17250}p_{0,2} + \tfrac{46821}{11500}p_{1,1} - \tfrac{1}{2}p_{1,0} \right)\varepsilon^2 - f_{1,2}.
\end{aligned}$$

The coefficients are plotted as functions of ε in the left part of Figure 4 for the function

$$f_3(\underline{x}) = \frac{25}{25 + (x - 1/5)^2 + 2y^2}.$$

For all the coefficients of the third order terms, the optimal ε is either at $\varepsilon = 0$ or on the imaginary axis in the ε-plane. The fourth order terms have optima on the real axis given by The approximate error $e_1(\underline{x}, \varepsilon)$ for $N = 6$ is shown in Figure 4 together with the computed errors for $N = 6$, 10, 15, and 21 points, corresponding to $K = 2$, 3, 4, and 5. The agreement between the approximation and the computed error is excellent. The global minimum is a compromise located at $\varepsilon^* \approx 0.2$.

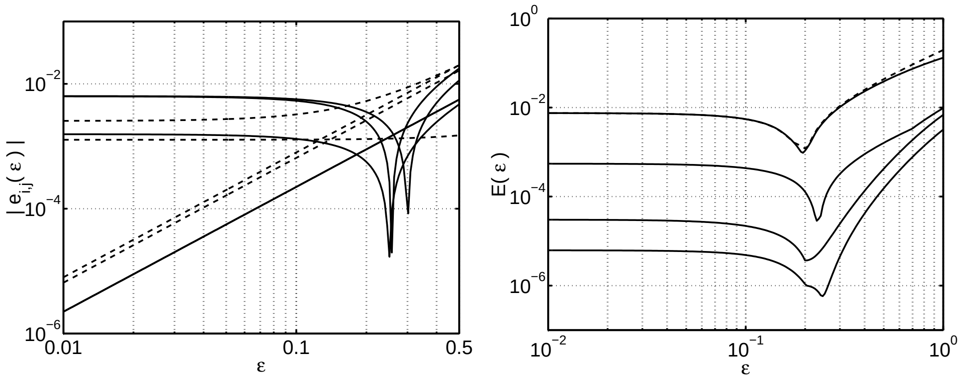


Figure 4: The left part of the figure shows the coefficients $e_j(\varepsilon)$ for terms with $|j| = 4$ (solid lines) and $|j| = 3$ (dashed lines) in the approximate error $\tilde{e}_1(\underline{x}, \varepsilon)$. To the right, the computed error (solid lines) for $N = 6$, 10, 15, and 21 points is displayed. The dashed line shows the approximation $\tilde{e}_1(\underline{x}, \varepsilon)$ for $N = 6$.

The example shows that the situation is much more complicated in two (and more) space dimensions. For each individual term, the best ε is governed by the decay rate of the Taylor expansion of the solution function, but many different terms contribute to the error and it is hard to make them all small at the same time. Still, there is usually a best choice of shape parameter. Exactly where the optimum is located depends on a compound function of decay rates of the coefficients in the Taylor expansion and also, to a larger extent than in 1D, on the placement of the node points.

However, the general properties given for the one-dimensional case in the previous subsection hold also for two and more dimensions. As can be seen in the right part of Figure 4, the error curves are very similar to those obtained for the one-dimensional problems.

7.4 The polynomial case

As mentioned previously in Section 7.1 and implicitly in Theorem 4.1, $\varepsilon = 0$ leads to the exact solution if the given data is polynomial and of degree $\leq K$. If the data has degree $K - Q$, then the error is of order $\varepsilon^{2\lfloor \frac{Q}{2} \rfloor + 2}$. This is illustrated in Figure 5 for the functions

$$\begin{aligned} f_4(x) &= 1 + x + x^2 \\ f_5(x, y) &= 1 + x - 2y + x^2 - xy + 2y^2 \end{aligned}$$

in one and two space dimensions respectively. For the one-dimensional problem, the number of points used are $N = 3, \ldots, 10$, corresponding with $K = 2, \ldots, 9$. In the two-dimensional case, $N = 6$, 10, 15, 21, 28, and 36 corresponding with $K = 2, \ldots, 7$.

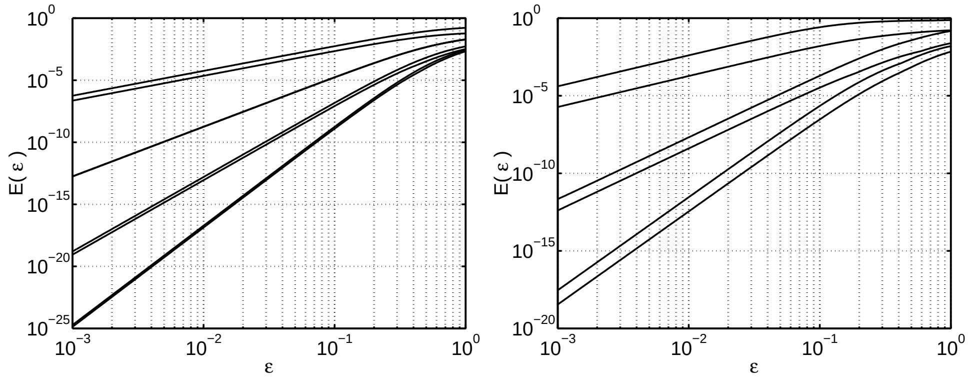


Figure 5: The computed error for the functions $f_4(x)$ (left) and $f_5(\underline{x})$ (right) using MQ RBFs and different numbers of points.

8 Conclusions

In this paper, we have studied RBF interpolation of smooth functions. We have focussed on the limit of nearly flat RBFs and given explicit expressions for the form of the (multivariate) interpolants in the limit region in terms of the shape parameter. In order for the limits to have the given form, the RBF must fulfill certain criteria, but as far as we can determine, these criteria hold for all of the standard RBFs in use.

We have used the results for the limits to analyze how the interpolation error depends on the shape parameter ε and we were able to explain why the error curve very often has a global minimum for some small nonzero value of ε. We could also explain which factors influence the optimal shape parameter value and in what way.

References

[1] R. L. Hardy, Multiquadric equations of topography and other irregular surfaces. *J. Geophys. Res.* **76** 1905–1915 (1971).

[2] R. L. Hardy, Theory and applications of the multiquadric-biharmonic method. 20 years of discovery 1968–1988. *Computers Math. Applic.* **19** (8-9) 163–208 (1990).

[3] M. J. D. Powell, The theory of radial basis function approximation in 1990, in *Advances in numerical analysis, Vol. II (Lancaster, 1990)*, pp. 105–210, Oxford Univ. Press, New York (1992).

[4] E. J. Kansa, Multiquadrics—A scattered data approximation scheme with applications to computational fluid-dynamics. II. Solutions to parabolic, hyperbolic and elliptic partial differential equations. *Computers Math. Applic.* **19** (8/9) 147–161 (1990).

[5] Z. M. Wu, Hermite-Birkhoff interpolation of scattered data by radial basis functions. *Approx. Theory Appl.* **8** (2) 1–10 (1992).

[6] G. E. Fasshauer, Solving partial differential equations by collocation with radial basis functions, in *Surface fitting and multiresolution methods (Chamonix–Mont-Blanc, 1996)* (Edited by A. Le Méhauté, C. Rabut, and L. L. Schumaker), pp. 131–138, Vanderbilt University Press, Nashville, TN (1997).

[7] Z. Wu, Solving differential equations with radial basis functions, in *Advances in computational mathematics (Guangzhou, 1997)*, pp. 537–543, Dekker, New York (1999).

[8] G. E. Fasshauer, Solving differential equations with radial basis functions: multilevel methods and smoothing. *Adv. Comput. Math.* **11** (2-3) 139–159 (1999), Radial basis functions and their applications.

[9] C. Franke and R. Schaback, Solving partial differential equations by collocation using radial basis functions. *Appl. Math. Comput.* **93** (1) 73–82 (1998).

[10] A. I. Fedoseyev, M. J. Friedman, and E. J. Kansa, Improved multiquadric method for elliptic partial differential equations via PDE collocation on the boundary. *Computers Math. Applic.* **43** (3–5) 439–455 (2002).

[11] E. Larsson and B. Fornberg, A numerical study of some radial basis function based solution methods for elliptic PDEs. *Computers Math. Applic.* (2003), to appear.

[12] F. J. Narcowich, R. Schaback, and J. D. Ward, Multilevel interpolation and approximation. *Appl. Comput. Harmon. Anal.* **7** (3) 243–261 (1999).

[13] E. J. Kansa and Y. C. Hon, Circumventing the ill-conditioning problem with multiquadric radial basis functions: applications to elliptic partial differential equations. *Computers Math. Applic.* **39** (7-8) 123–137 (2000).

[14] R. K. Beatson, W. A. Light, and S. Billings, Fast solution of the radial basis function interpolation equations: domain decomposition methods. *SIAM J. Sci. Comput.* **22** (5) 1717–1740 (2000).

[15] J. B. Cherrie, R. K. Beatson, and G. N. Newsam, Fast evaluation of radial basis functions: methods for generalized multiquadrics in $\mathbb{R}^n$. *SIAM J. Sci. Comput.* **23** (5) 1549–1571 (2002).

[16] B. Fornberg and G. Wright, Stable computation of multiquadric interpolants for all values of the shape parameter. Submitted to *Computers Math. Applic.* (2002).

[17] R. Schaback, Improved error bounds for scattered data interpolation by radial basis functions. *Math. Comp.* **68** (225) 201–216 (1999).

[18] A. Bejancu, Jr., Local accuracy for radial basis function interpolation on finite uniform grids. *J. Approx. Theory* **99** (2) 242–257 (1999).

[19] W. R. Madych, Miscellaneous error bounds for multiquadric and related interpolators. *Computers Math. Applic.* **24** (12) 121–138 (1992).

[20] M. Buhmann and N. Dyn, Spectral convergence of multiquadric interpolation. *Proc. Edinburgh Math. Soc. (2)* **36** (2) 319–333 (1993).

[21] B. Fornberg, G. Wright, and E. Larsson, Some observations regarding interpolants in the limit of flat radial basis functions. *Comput. Math. Appl.* (2003), to appear.

[22] T. A. Driscoll and B. Fornberg, Interpolation in the limit of increasingly flat radial basis functions. *Computers Math. Applic.* **43** (3–5) 413–422 (2002).

[23] R. Schaback, Multivariate interpolation by polynomials and radial basis functions. Preprint (2002).

[24] R. J. Y. McLeod and M. L. Baart, *Geometry and interpolation of curves and surfaces*, Cambridge University Press, Cambridge (1998).

[25] W. R. Madych and S. A. Nelson, Bounds on multivariate polynomials and exponential error estimates for multiquadric interpolation. *J. Approx. Theory* **70** (1) 94–114 (1992).

[26] A. H.-D. Cheng, M. A. Golberg, E. J. Kansa, and G. Zammito, Exponential convergence and H-c multiquadric collocation method for partial differential equations. *Numer. Methods Partial Differential Equations* **19** (5) 571–594 (2003).

[27] R. E. Carlson and T. A. Foley, The parameter R^2 in multiquadric interpolation. *Computers Math. Applic.* **21** (9) 29–42 (1991).

[28] M. A. Golberg, C. S. Chen, and S. R. Karur, Improved multiquadric approximation for partial differential equations. *Engng. Anal. Bound. Elem.* **18** (1) 9–17 (1996).

[29] S. Rippa, An algorithm for selecting a good value for the parameter c in radial basis function interpolation. *Adv. Comput. Math.* **11** (2-3) 193–210 (1999).

[30] Z. M. Wu and R. Schaback, Local error estimates for radial basis function interpolation of scattered data. *IMA J. Numer. Anal.* **13** (1) 13–27 (1993).