The Mystery of the Shape Parameter III

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Abstract. This is a continuation of our earlier study of the shape parameter \( c \) contained in the famous multiquadrics \((-1)^{\beta} (c^2 + \|x\|^2)^\beta, \beta > 0\), and the inverse multiquadrics \((c^2 + \|x\|^2)^\beta, \beta < 0\).

In \cite{9} and \cite{10} we present criteria for the optimal choice of \( c \), based on the exponential-type error bound\cite{6}. In this paper a new set of criteria is developed, based on the improved exponential-type error bound\cite{7}. Unlike \cite{9} and \cite{10}, where the range of \( c \) is only a subset of \((0, \infty)\), the range of \( c \) we investigate here is the entire interval \((0, \infty)\). The drawback is that the distribution of the data points is not purely scattered. However it seems to be harmless.

Key words: radial basis function, multiquadric, shape parameter, interpolation

1 Introduction

We begin with some basic ingredients of our theoretical ground.

Let \( T_n \) denote the \( n \)-simplex in \( R^n \) whose definition can be found in \cite{3}. A 1-simplex is a line segment, a 2-simplex is a triangle, and a 3-simplex is a tetrahedron with four vertices.

Let \( v_i, 1 \leq i \leq n + 1 \) be the vertices of \( T_n \). Then any point \( x \in T_n \) can be written as convex combination of the vertices:

\[
x = \sum_{i=1}^{n+1} c_i v_i, \quad \sum_{i=1}^{n+1} c_i = 1, \quad c_i \geq 0.
\]

The numbers \( c_1, \ldots, c_{n+1} \) are called the barycentric coordinates of \( x \).

For any \( n \)-simplex \( T_n \), the evenly spaced points of degree \( l \) are those points whose barycentric coordinates are of the form

\[
\left( \frac{k_1}{l}, \frac{k_2}{l}, \ldots, \frac{k_{n+1}}{l} \right), \quad k_i \text{ nonnegative integers with } \sum_{i=1}^{n+1} k_i = l.
\]

If we let \( P^n_l \) denote the space of polynomials of degree not exceeding \( l \) in \( n \) variables, it’s easily seen that the number of evenly spaced points of degree \( l \) is exactly \( N = dim P^n_l = \binom{n+l}{n} \). Also, such points form a determining set for \( P^n_l \), by \cite{2}.

In this paper the interpolation will happen in \( n \)-simplex and the set \( X \) of centers(interpolation points) will be the evenly spaced points in the \( n \)-simplex.
The radial function we use is

\[ h(x) := \Gamma(-\frac{\beta^2}{2})(c^2 + \|x\|^2)^{\frac{\beta^2}{2}}, \beta \in \mathbb{R} \setminus 2\mathbb{N} \geq 0, \ c > 0 \]

(1)

where \( \|x\| \) is the Euclidean norm of \( x \in \mathbb{R}^n \), \( \Gamma \) is the classical gamma function, and \( \beta, c \) are constants. Note that this definition is slightly different from the one mentioned in the abstract. We adopt (1) because it will greatly simplify its Fourier transform and our future work. The function \( h(x) \) in (1) is conditionally positive definite (c.p.d.) of order \( m = \max\{0, \lceil \frac{\beta^2}{2} \rceil \} \) where \( \lceil \cdot \rceil \) means the smallest integer greater than or equal to \( \cdot \). Further details can be found in [11].

Given data points \((x_j, y_j), j = 1, \ldots, N\), where \( X = \{x_1, \ldots, x_N\} \) is a subset of \( \mathbb{R}^n \) and \( y_j \)'s are real or complex numbers, our interpolant will be of the form

\[ s(x) = p(x) + \sum_{j=1}^{N} c_j h(x - x_j) \]

(2)

where \( p(x) \) is a polynomial in \( P_{m-1}^n \) to be determined and \( c_j \)'s are coefficients to be chosen.

As is well known in the theory of radial basis functions, if \( X \) is a determining set for \( P_{m-1}^n \), there exists a unique polynomial \( p(x) \) and unique constants \( c_1, \ldots, c_N \) satisfying the linear system

\[ p(x_i) + \sum_{j=1}^{N} c_j h(x_i - x_j) = y_i, \ i = 1, \ldots, N \]

(3)

\[ \sum_{j=1}^{N} c_j q(x_j) = 0 \]

where \( q \) ranges over all basis elements of \( P_{m-1}^n \). All these can be found in [11].

1.1 Fundamental theory

Each function \( h \) of the form (1) induces a function space \( C_{h,m} \), called native space, whose definition and characterization can be found in [11], [12], [11], [13], [8], and [14]. Here \( m = \max\{0, \lceil \frac{\beta^2}{2} \rceil \} \). Also, there is a seminorm \( \|f\|_h \) for each \( f \in C_{h,m} \). In our theory every interpolated function belongs to the native space.

Before entering the main theorem, let’s introduce two constants.

Definition 1.1 Let \( n \) and \( \beta \) be as in (1). The numbers \( \rho \) and \( \Delta_0 \) are defined as follows.

(a) Suppose \( \beta < n - 3 \). Let \( s = \lceil \frac{n-\beta-3}{2} \rceil \). Then

(i) if \( \beta < 0 \), \( \rho = \frac{3+s}{3} \) and \( \Delta_0 = \frac{(2+s)(1+s)-3}{\rho^s} \);

(ii) if \( \beta > 0 \), \( \rho = 1 + \frac{s}{2\lceil \frac{\beta}{2} \rceil +3} \) and \( \Delta_0 = \frac{(2m+2+s)(2m+1+s)\cdots(2m+3)}{\rho^{m+s+2}} \)

where \( m = \lceil \frac{\beta}{2} \rceil \).

(b) Suppose \( n - 3 \leq \beta < n - 1 \). Then \( \rho = 1 \) and \( \Delta_0 = 1 \).

(c) Suppose \( \beta \geq n - 1 \). Let \( s = -\lceil \frac{n-\beta-3}{2} \rceil \). Then

\[ \rho = 1 \text{ and } \Delta_0 = \frac{1}{(2m+2)(2m+1)\cdots(2m-s+3)} \text{ where } m = \lceil \frac{\beta}{2} \rceil. \]

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Our criteria for the optimal choice of $c$ is based on the following theorem which we cite directly from [7] but with a slight modification to make it easier to understand.

**Theorem 1.2** Let $h$ be as in (1). For any positive number $b_0$, let $C = \max\{\frac{2}{3C\delta}, 8\rho\}$ and $\delta_0 = \frac{1}{3C\delta}$.

For any $n$-simplex $Q$ of diameter $r$ satisfying $\frac{1}{\sqrt{3C\delta}} \leq r \leq \frac{2}{\sqrt{3C\delta}}$ (note that $\frac{1}{\sqrt{3C\delta}} \leq b_0$), if $f \in C_{h,m}$,

$$ |f(x) - s(x)| \leq 2^{n-\frac{n-\beta}{2} + n-\frac{1}{2} + \frac{1}{2} - l} \sqrt{\alpha_0} \sqrt{3C} \sqrt{\delta(\lambda')} \|f\|_h $$

(4)

holds for all $x \in Q$ and $0 < \delta < \delta_0$, where $s(x)$ is defined as in (2) with $x_1, \ldots, x_N$ the evenly spaced points of degree $l$ in $Q$ satisfying $\frac{1}{3C\delta} \leq l \leq \frac{2}{3C\delta}$. The constant $\alpha_n$ denotes the volume of the unit ball in $R^n$, and $0 < \lambda' < 1$ is given by

$$ \lambda' = \left(\frac{2\pi}{3}\right)^{\frac{m}{n}} $$

which only in some cases mildly depends on the dimension $n$.

**Remark:** This seemingly complicated theorem is in fact not difficult to understand. Note that the right-hand side of (4) approaches zero as $\delta$ tends to zero. Also, (4) is greatly influenced by the shape parameter $c$. However, in order to make it useful in the choice of $c$, we still have to do some work.

We begin with the following definition.

**Definition 1.3** For any $\sigma > 0$, the class of band-limited functions $f$ in $L^2(R^n)$ is defined by

$$ B_{\sigma} = \{f \in L^2(R^n) : \hat{f}(\xi) = 0 \text{ if } |\xi| > \sigma\} $$

, where $\hat{f}$ denotes the Fourier transform of $f$.

Now we cite Theorem 1.6 of [9] as a lemma.

**Lemma 1.4** Let $h$ be as in (1) with $\beta > 0$. Any function $f$ in $B_{\sigma}$ belongs to $C_{h,m}$ and

$$ \|f\|_h \leq \sqrt{m!S(m,n)} 2^{-n-\frac{1+\beta}{4}} \pi^{-\frac{1}{2}} \sigma e^{\frac{1}{2}} e^{\frac{1}{2} - \frac{1}{2} - n} \|f\|_{L^2(R^n)} $$

where $c, \beta$ are as in (1) and $S(m,n)$ is a constant determined by $m$ and $n$.

**Corollary 1.5** Let $h$ be as in (1) with $\beta > 0$. If $\sigma > 0$ and $f \in B_{\sigma}$, the inequality (4) can be transformed into

$$ |f(x) - s(x)| \leq 2^{2-\frac{n}{2} - 3n} \sqrt{\alpha_0 \sqrt{3C}} \sqrt{m!S(m,n)} \sigma e^{\frac{1+\beta+n}{4}} e^{\frac{1+\beta+n}{4} - l} e^{\frac{1+\beta+n}{4} - l} \sqrt{3}(\lambda') \|f\|_{L^2(R^n)} $$

(5)

In order to handle the case $\beta < 0$, we need the following lemma which is just Theorem 1.7 of [9].

**Lemma 1.6** Let $h$ be as in (1) with $\beta < 0$ such that $n + \beta \geq 1$ or $n + \beta = -1$. Any function $f$ in $B_{\sigma}$ belongs to $C_{h,m}$ and satisfies

$$ \|f\|_h \leq 2^{-n-\frac{1+\beta}{4}} \pi^{-\frac{1}{2}} \sigma e^{\frac{1}{2}} e^{\frac{1}{2} - \frac{1}{2} - n} \|f\|_{L^2(R^n)} $$

**Corollary 1.7** Let $h$ be as in (1) with $\beta < 0$ such that $n + \beta \geq 1$ or $n + \beta = -1$. If $\sigma > 0$ and $f \in B_{\sigma}$, the inequality (4) can be transformed into

$$ |f(x) - s(x)| \leq 2^{2-\frac{n}{2} - 3n} \sqrt{\alpha_0 \sqrt{3C}} \sqrt{m!S(m,n)} \sigma e^{\frac{1+\beta+n}{4}} e^{\frac{1+\beta+n}{4} - l} e^{\frac{1+\beta+n}{4} - l} \sqrt{3}(\lambda') \|f\|_{L^2(R^n)} $$

(6)
Note that Corollary 1.7 does not cover the frequently seen case $\beta = -1, n = 1$. For this we need the following lemma which is just Lemma 2.1 of [9].

**Lemma 1.8** Let $h$ be as in (1) with $\beta = -1, n = 1$. For any $\sigma > 0$, if $f \in B_\sigma$, then $f \in C_{h,m}$ and

$$
\|f\|_h \leq (2\pi)^{-n/2} \left\{ \frac{1}{\mathcal{K}_0(1)} \int_{|\xi| \leq \frac{c}{4}} |\hat{f}(\xi)|^2 d\xi + \frac{1}{a_0} \int_{\frac{c}{4} < |\xi| \leq c} |\hat{f}(\xi)|^2 \sqrt{c|\xi|e^{c|\xi|}} d\xi \right\}^{1/2}
$$

if $\frac{1}{c} < \sigma$, where $a_0 = \frac{1}{2\sqrt{3}}$, and

$$
\|f\|_h \leq (2\pi)^{-n/2} \left\{ \frac{1}{\mathcal{K}_0(1)} \int_{|\xi| \leq \frac{c}{4}} |\hat{f}(\xi)|^2 d\xi \right\}^{1/2}
$$

if $\frac{1}{c} \geq \sigma$.

**Corollary 1.9** Let $h$ be as in (1) with $\beta = -1, n = 1$. If $\sigma > 0$ and $f \in B_\sigma$, the inequality (4) can be transformed into

$$
|f(x) - s(x)| \leq 2^{-2+\frac{3n+4}{2}} \frac{\pi^{-\frac{3n+1}{2}}}{n!} \sqrt{\Delta_0} \sqrt{3Ce^{2\lambda}} \left( A + B \right)^{1/2} (7)
$$

where $A = \frac{1}{\mathcal{K}_0(1)} \int_{|\xi| \leq \frac{c}{4}} |\hat{f}(\xi)|^2 d\xi$ for all $c$, $B = 2\sqrt{3} \int_{\frac{c}{4} < |\xi| \leq c} |\hat{f}(\xi)|^2 \sqrt{c|\xi|e^{c|\xi|}} d\xi$ if $\frac{1}{c} < \sigma$, and $B = 0$ if $\frac{1}{c} \geq \sigma$.

### 2 Criteria of Choosing $c$

The results of Section 1 provide us with useful theoretical ground for choosing $c$. Note that in the right-hand side of (5), (6) and (7), there is always a main function determined by $c$. Let’s call it the MN function, denoted by $MN(c)$, as in [10]. Its graph is called MN curve. Then finding the optimal value of $c$ is equivalent to finding the minimum of $MN(c)$. Let’s analyze as follows. Here the range of $c$ is the entire interval $(0, \infty)$.

#### Case 1. $\beta > 0$ and $n \geq 1$

Let $f \in B_\sigma$ and $h$ be defined as in (1) with $\beta > 0$ and $n \geq 1$. Under the conditions of Theorem 1.2, for any fixed $\delta$ satisfying $0 < \delta < \delta_0$, the optimal choice of $c$ is as follows.

(a) If $1 + \beta - n - 4l \geq 0$, where $l$ is defined as in Theorem 1.2, let $c$ be as small as possible.

(b) If $1 + \beta - n - 4l < 0$, where $l$ is defined as in Theorem 1.2, the optimal $c$ is where the minimum of $MN(c) := e^{\frac{\pi^2}{2}} c^{\frac{1+\beta-n-4l}{2}}$ occurs.

**Reason:** (a) By (5) the MN function is $MN(c) = e^{\frac{\pi^2}{2}} c^{\frac{1+\beta-n-4l}{2}}$. If $1 + \beta - n - 4l \geq 0$, $MN(c)$ is an increasing function. Hence the smaller $c$ is, the better it is. (b) If $1 + \beta - n - 4l < 0$, $MN(c) \to \infty$ both as $c \to 0^+$ and $c \to \infty$. The minimum of $MN(c)$ corresponds to the optimal choice of $c$ because it makes the error bound (5) minimum.

**Remark:** For (b), the optimal $c$ can be easily found by Mathematica or Matlab.

**Numerical Results:**
Graph of the MN Curve with $\delta=0.01$ and $l=5$

Figure 1: Here $n = 1$, $\beta = 1$, $b_0 = 1$ and $\sigma = 1$.

Graph of the MN Curve with $\delta=0.008$ and $l=6$

Figure 2: Here $n = 1$, $\beta = 1$, $b_0 = 1$ and $\sigma = 1$.

Graph of the MN Curve with $\delta=0.006$ and $l=7$

Figure 3: Here $n = 1$, $\beta = 1$, $b_0 = 1$ and $\sigma = 1$. 
For $\beta < 0$, we separate it into two cases.

**Case 2.** $\beta < 0$ and $n + \beta \geq 1$ or $n + \beta = -1$. Let $f \in \mathcal{B}_\sigma$ and $h$ be defined as in (1) with $\beta < 0$ and $n + \beta \geq 1$, or $n + \beta = -1$. Under the conditions of Theorem 1.2, for any fixed $\delta$ satisfying $0 < \delta < \delta_0$, the optimal value of $c$ is the number minimizing $MN(c) := e^{\frac{c}{2\sigma}} e^{\frac{1+\beta-n-4l}{4}}$ where $l$ is defined as in Theorem 1.2.

**Reason:** This is an immediate result of Corollary 1.7. Note that in this case $1 + \beta - n - 4l$ is always negative. So $MN(c) \to \infty$ both as $c \to 0^+$ and $c \to \infty$.

**Remark:** Case 2 covers $\beta = -1$ and $n \geq 2$.

**Numerical Results:**
Figure 6: Here $n = 2$, $\beta = -1$, $b_0 = 1$ and $\sigma = 1$.

Figure 7: Here $n = 2$, $\beta = -1$, $b_0 = 1$ and $\sigma = 1$.

Figure 8: Here $n = 2$, $\beta = -1$, $b_0 = 1$ and $\sigma = 1$. 
Now we begin the case $\beta = -1$ and $n = 1$.

**Case 3.** $\beta = -1$ and $n = 1$  Let $f \in B_\sigma$ and $h$ be defined as in (1) with $\beta = -1$ and $n = 1$. Under the conditions of Theorem 1.2, for any fixed $\delta$ satisfying $0 < \delta < \delta_0$, the optimal value of $c$ is the number minimizing $MN(c)$, defined by

$$
MN(c) := \begin{cases} 
\frac{1}{\sqrt{K_0(1)}}c^{\frac{1}{2}} - l & \text{if } 0 < c \leq \frac{1}{\sigma}, \\
c^{\frac{1}{2}} - l \left[ \frac{1}{K_0(1)} + 2\sqrt{3\sqrt{c}\sigma e^{c\sigma}} \right]^{1/2} & \text{if } \frac{1}{\sigma} < c
\end{cases}
$$

, where $l$ is defined as in Theorem 1.2 and $K_0$ is the modified Bessel function.

**Reason:** In (7), the part of the upper bound influenced by $c$ is $c^{\frac{1}{2}} - l \left[ \frac{1}{K_0(1)} + 2\sqrt{3\sqrt{c}\sigma e^{c\sigma}} \right]^{1/2}$. Note that for $0 < c \leq \frac{1}{\sigma}$, we have $\sigma \leq \frac{1}{c}$ and

$$
A = \frac{1}{K_0(1)} \int_{|\xi| \leq \frac{1}{c}} |\hat{f}(\xi)|^2 d\xi = \frac{1}{K_0(1)} \int_{|\xi| \leq \sigma} |\hat{f}(\xi)|^2 d\xi = \frac{1}{K_0(1)} \|f\|^2_{L^2(R^n)}
$$
because $f \in B_\sigma$. Therefore

$$c^{\frac{d}{2} - 1} \{A + B\}^{\frac{1}{2}} = c^{\frac{d}{2} - 1} \sqrt{A} = \frac{1}{\sqrt{K_0(1)}} c^{\frac{d}{2} - 1} \|f\|_{L^2(\mathbb{R}^n)}$$

if $0 < c \leq \frac{1}{\sigma}$. Now, if $\frac{1}{\sigma} < c$,

$$c^{\frac{d}{2} - 1} \{A + B\}^{\frac{1}{2}} \leq c^{\frac{d}{2} - 1} \left\{ \frac{1}{K_0(1)} \right\} \left\{ \int_{|\xi| \leq \sigma} |\hat{f}(\xi)|^2 d\xi + 2\sqrt{3} \int_{\frac{|\xi|}{c} \leq \sigma} |\hat{f}(\xi)|^2 \sqrt{c|\xi|} e^{\xi^T} d\xi \right\}^{1/2}$$

As a result, the MN function is

$$MN(c) := \begin{cases} 
\frac{1}{\sqrt{K_0(1)}} c^{\frac{d}{2} - 1} & \text{if } 0 < c \leq \frac{1}{\sigma}, \\
\|f\|_{L^2(\mathbb{R}^n)} + 2\sqrt{3} \|c\| e^{\sigma} \|f\|_{L^2(\mathbb{R}^n)} & \text{if } \frac{1}{\sigma} < c.
\end{cases}$$

Numerical Results:

Graph of the MN Curve with $\delta=0.01$ and $l=5$

Figure 11: Here $n = 1$, $\beta = -1$, $b_0 = 1$ and $\sigma = 1$. 

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Figure 12: Here $n = 1$, $\beta = -1$, $b_0 = 1$ and $\sigma = 1$.

Graph of the MN Curve with $\delta = 0.008$ and $l = 6$

Figure 13: Here $n = 1$, $\beta = -1$, $b_0 = 1$ and $\sigma = 1$.

Graph of the MN Curve with $\delta = 0.006$ and $l = 7$

Figure 14: Here $n = 1$, $\beta = -1$, $b_0 = 1$ and $\sigma = 1$. 
Note that the optimal $c$ increases rapidly as $\delta$ becomes small.

**Final Remark:** Both [9] and this paper deal with the interpolation of band-limited functions. In [9] the range of $c$ is $[12\rho \sqrt{\pi} e^{2\pi^2} \gamma_n (m + 1) \delta, \infty)$ and is only a subset of $(0, \infty)$. In order to make the left endpoint of the closed-open interval small enough, often $\delta$ must be very small. The consequence is that a huge number of data points will be involved, making the criteria of choosing $c$ only theoretically valuable, especially for $n \geq 2$. Now we have thoroughly removed this restriction. In this paper the range of $c$ is $(0, \infty)$.

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