Multiquadric and Its Shape Parameter—A Numerical Investigation of Error Estimate, Condition Number, and Round-Off Error by Arbitrary Precision Computation

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Objectives

- Explore the theoretical result on RBF collocation by numerical experiment.
- The tool used is arbitrary precision computation.

- Issues examined include:
  - Positive definiteness
  - Error estimate with respect to fill distance
  - Infinitely flat shape parameter
  - Error estimate with respect to shape parameter
  - Optimal shape parameter
  - Condition number
  - Effective condition number
  - Round off error
  - Edge effect
  - Error estimate on derivative data and PDE

Example: Madych's Error Estimate

For a class of interpolators that include GA, MQ and IMQ, Madych provided the following error estimates: for $f \in B_\sigma$,

$$\varepsilon \sim O\left(e^{ac}\lambda^{c/h}\right), \quad \text{for} \quad 0 < \lambda < 1 \quad \text{and} \quad a > 0 \tag{47}$$

and for $f \in E_\sigma$,

$$\varepsilon \sim O\left(e^{ac^2}\lambda^{c/h}\right), \quad \text{for} \quad 0 < \lambda < 1 \quad \text{and} \quad a > 0 \tag{48}$$

We observe that these error estimates are made of the product of two competing terms as c becomes large—one part grows exponentially, and the other decays exponentially.

Empirical Error Estimate

- IMQ

$$\varepsilon \sim O\left(e^{ac^{3/2}} \lambda^{c^{1/2}/h}\right), \quad \text{for} \quad 0<\lambda<1 \quad \text{and} \quad a>0$$

- Gaussian

$$\varepsilon \sim O\left(e^{ac^{4}} \lambda^{c/h}\right), \quad \text{for} \quad 0<\lambda<1 \quad \text{and} \quad a>0$$

RBF COLLOCATION METHOD

Approximation of Function

- Problem statement: Approximate a function $f(\mathbf{x})$, using the following series

$$f(\mathbf{x}) \approx \hat{f}(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i \varphi(r_i); \quad r_i = \left\| \mathbf{x}_i - \mathbf{x} \right\|$$

- where $\varphi(r_i)$ is a radial basis (distance) function
- Method of solution: Select a set of locations,

  $\mathbf{x}_j,\ j = 1, \ldots, n$, and require

$$\hat{f}(\mathbf{x}_j) = \sum_{i=1}^{n} \alpha_i \varphi_i(\mathbf{x}_j) = f(\mathbf{x}_j); \quad j = 1, \ldots, n$$

Solution of PDE (Collocation Using Derivative Data)

- Problem statement: Find $f(\mathbf{x})$ that (approximately) satisfies

$$L\{f(\mathbf{x})\} = g(\mathbf{x}), \quad \mathbf{x} \in \Omega;$$

$$B\{f(\mathbf{x})\} = b(\mathbf{x}), \quad \mathbf{x} \in \Gamma;$$

- Method of solution: approximate $f(\mathbf{x})$ as

$$f(\mathbf{x}) \approx \hat{f}(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i \varphi(r_i); \quad r_i = \|\mathbf{x}_i - \mathbf{x}\|$$

Collocation

- Require

$$L\{\hat{f}(\mathbf{x}_j)\} = L\{\sum_{i=1}^{n} \alpha_i \varphi(r_{ij})\} = \sum_{i=1}^{n} \alpha_i L\{\varphi(r_{ij})\} = \sum_{i=1}^{n} \alpha_i L_{ij} = g(\mathbf{x}_j),$$

$$\mathbf{x}_j \in \Omega; \quad j = 1, \ldots, n_1$$

$$B\{\hat{f}(\mathbf{x}_j)\} = B\{\sum_{i=1}^{n} \alpha_i \varphi(r_{ij})\} = \sum_{i=1}^{n} \alpha_i B\{\varphi(r_{ij})\} = \sum_{i=1}^{n} \alpha_i B_{ij} = b(\mathbf{x}_j),$$

$$\mathbf{x}_j \in \Gamma; \quad j = n_1 + 1, \ldots, n$$

- Data is given not as the function itself, but as its derivates.

EXAMPLES OF RBF

Examples of RBF

- pseudo-polynomial (1-D and 2-D) and polyharmonic spline (3-D)

$$\varphi = r^{2k-1}; \quad k = 1,2,3,\ldots$$

- polyharmonic spline (1-D and 2-D)

$$\varphi = r^{2k} \ln r, \quad k = 1,2,3,\ldots$$

- generalized multiquadric [4, 37]

$$\varphi = \left(r^2 + c^2\right)^{k/2}, \; k \text{ is any real number } \neq 0,2,4,\ldots$$

- shifted logarithmic [24]

$$\varphi = \ln(r^2 + c^2)$$

- shifted polyharmonic spline

$$\varphi = (r^2 + c^2)^k \ln(r^2 + c^2), \quad k = 1, 2, 3, \ldots$$

- Gaussian

$$\varphi = e^{-r^2/c^2}$$

Schoenberg 1937

Schoenberg in 1937 [84] first demonstrated that if $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$ are a set of distinct data locations, then the interpolation matrix $[\mathbf{A}]$ for the conical RBF $\varphi = r$, with its elements $a_{ij} = r_{ij}$, is nonsingular and invertible.

Hardy's Multiquadric (1971)

- Multiquadric

$$\varphi = \sqrt{r^2 + c^2}$$

- Inverse multiquadric

$$\varphi = 1 \Big/ \sqrt{r^2 + c^2}$$

- Generalized multiquadric (Barnhill and Stead 1984)

$$\varphi_i = \left(r_i^2 + c^2\right)^{k/2}, \ k \text{ any real number } \neq 0,2,4,\ldots$$

Duchon Splines (1976)

- Minimize

$$I = \iint_S \left\| D^{2k} \hat{f}(\mathbf{x}) \right\| dx_1 dx_2$$

- Polyharmonic spline (2-D)

$$\varphi = r^{2k} \ln r, \quad k = 1, 2, 3, \ldots$$

- Pseudo-polynomials (3-D)

$$\varphi = r^{2k+1}; \quad k = 1, 2, 3, \ldots$$

Gaussian

- Used for interpolation since 1970s.
- Widely used in Neural Network since 1980's.

$$\varphi = e^{-r^2/c^2}$$

Franke (1982)

- Franke (1982) reported MQ as the best interpolation method, even outperforms thin plate spline, to the surprise of mathematicians.
- This article has set off a large number of mathematical investigation of RBF interpolation.

Micchelli (1986)

- Micchelli investigated the coefficient matrix of RBF interpolants with distinct centers, and proved the invertibility and conditionally positive definiteness of these matrices.

NUMERICAL EXPERIMENTS

Franke's Test Functions

$$f_1 = \frac{3}{4}\exp[-\frac{(9x-2)^2+(9y-2)^2}{4}] + \frac{3}{4}\exp[-\frac{(9x+1)^2}{49} - \frac{9y+1}{10}]$$
$$+ \frac{1}{2}\exp[-\frac{(9x-7)^2+(9y-3)^2}{4}] - \frac{1}{5}\exp[-(9x-4)^2-(9y-7)^2] \qquad (1)$$

$$f_2 = \frac{1}{9}\left[\tanh\left(9y-9x\right)+1\right] \qquad (2)$$

$$f_3 = \frac{1.25+\cos(5.4y)}{6[1+(3x-1)^2]} \qquad (3)$$

$$f_4 = \frac{1}{3}\exp\left\{-\frac{81}{16}\left[\left(x-\frac{1}{2}\right)^2+\left(y-\frac{1}{2}\right)^2\right]\right\} \qquad (4)$$

$$f_5 = \frac{1}{3}\exp\left\{-\frac{81}{4}\left[\left(x-\frac{1}{2}\right)^2+\left(y-\frac{1}{2}\right)^2\right]\right\} \qquad (5)$$

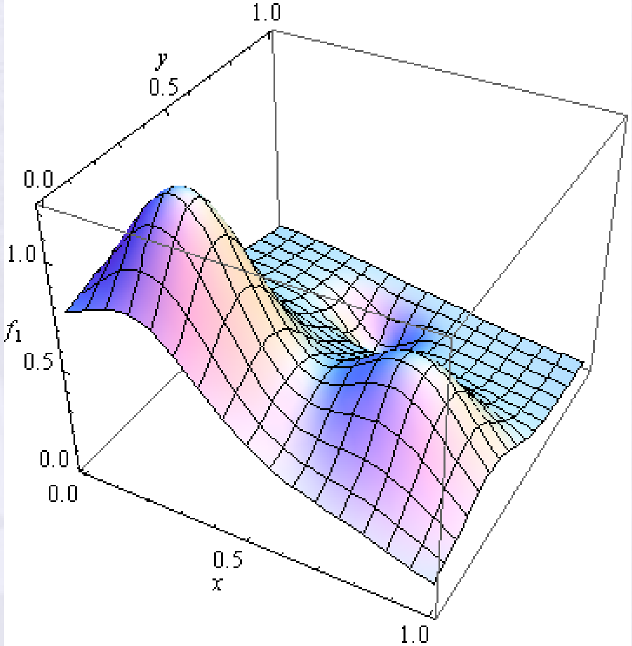
$$f_6 = \frac{1}{9}\left\{64-81\left[\left(x-\frac{1}{2}\right)^2+\left(y-\frac{1}{2}\right)^2\right]\right\}^{1/2} - \frac{1}{2} \qquad (6)$$

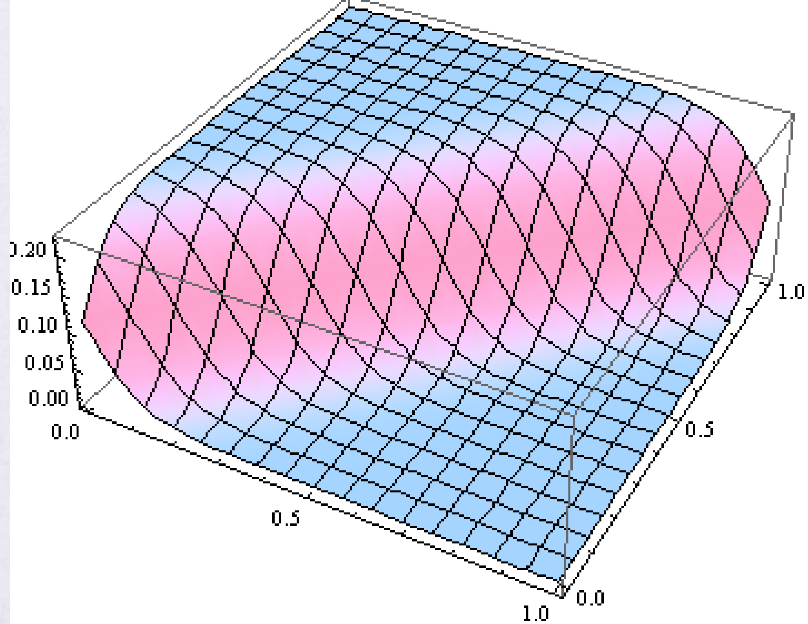
$$f_7 = 1+x+y \qquad (7)$$

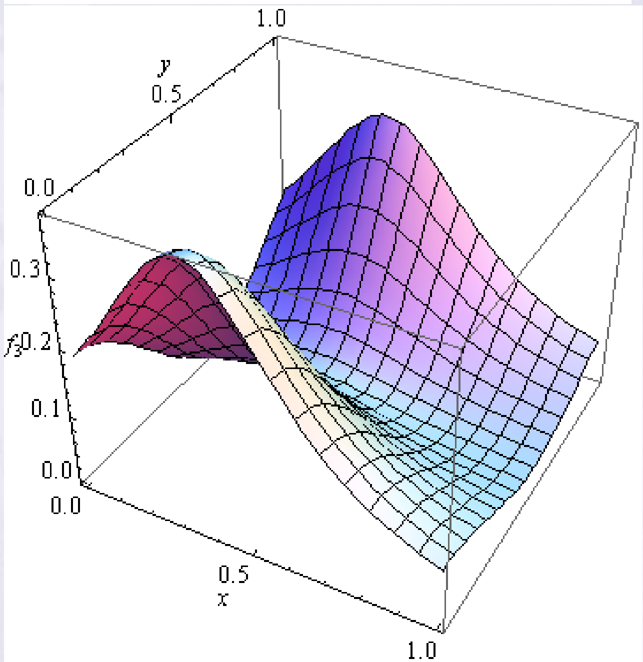
defined within $0 \le x \le 1$ and $0 \le y \le 1$.

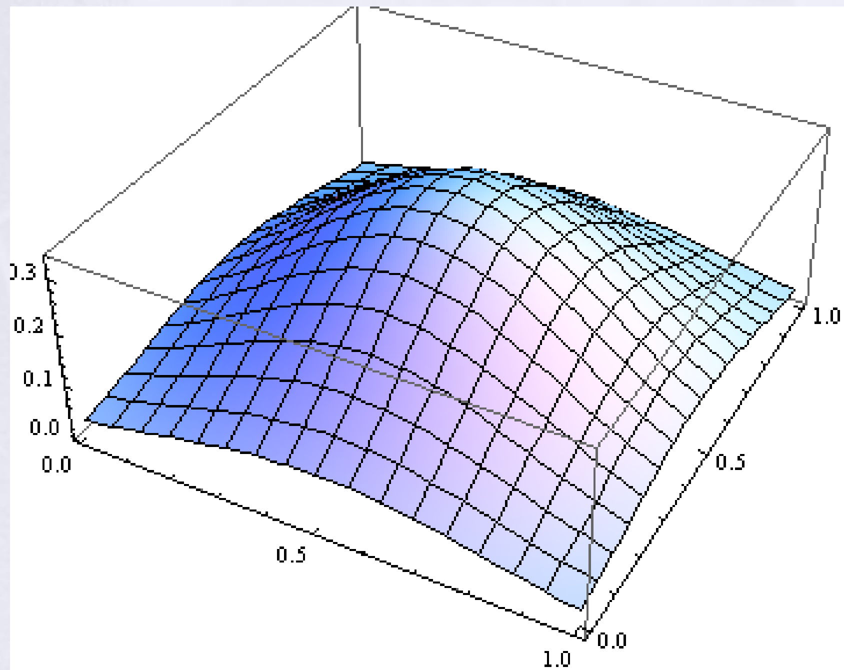
$$f_8 = \frac{\sin \pi x}{6} \frac{\sin 7\pi x}{4} \frac{\sin 3\pi y}{4} \frac{\sin 5\pi y}{4} \tag{1}$$

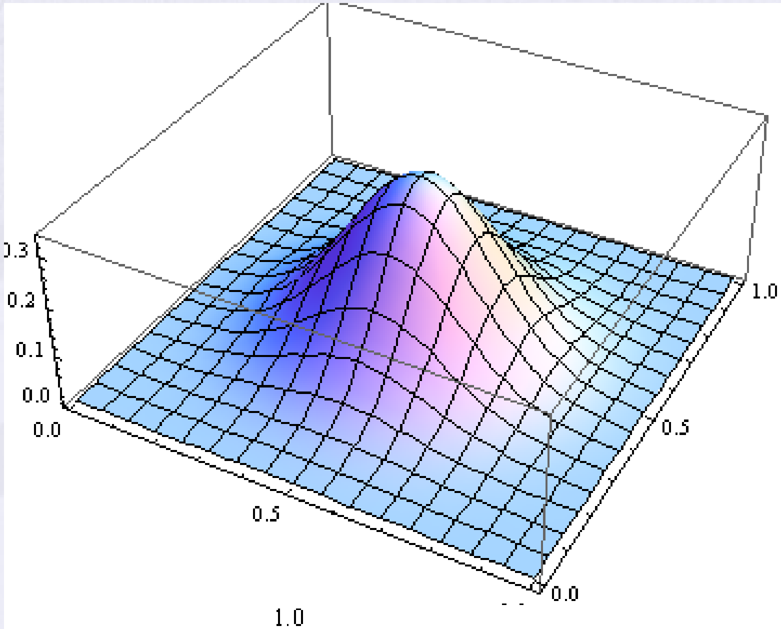
$$f_9 = \frac{\sin 2\pi x}{2\pi x} \frac{\sin 2\pi y}{2\pi y} \tag{2}$$


y
x
f_1




y
x
f_3

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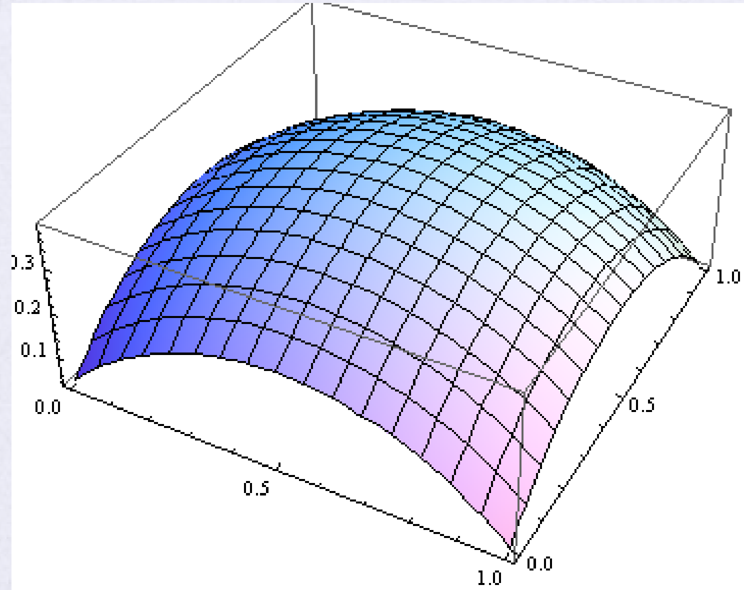
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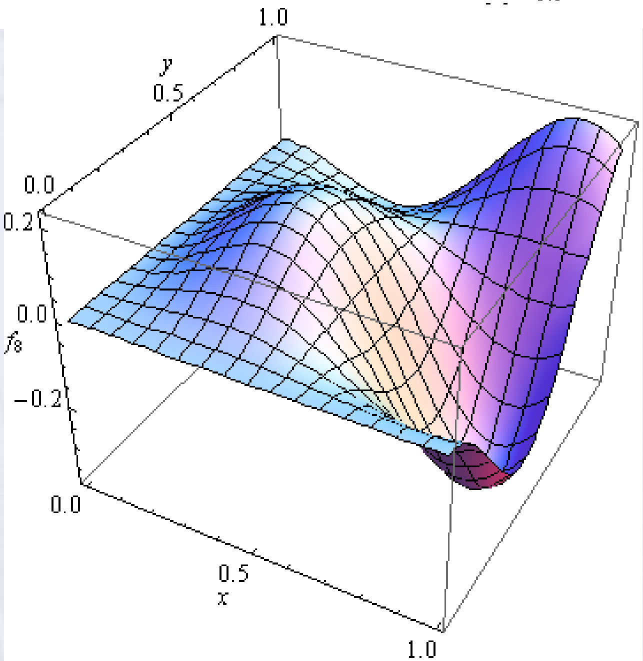
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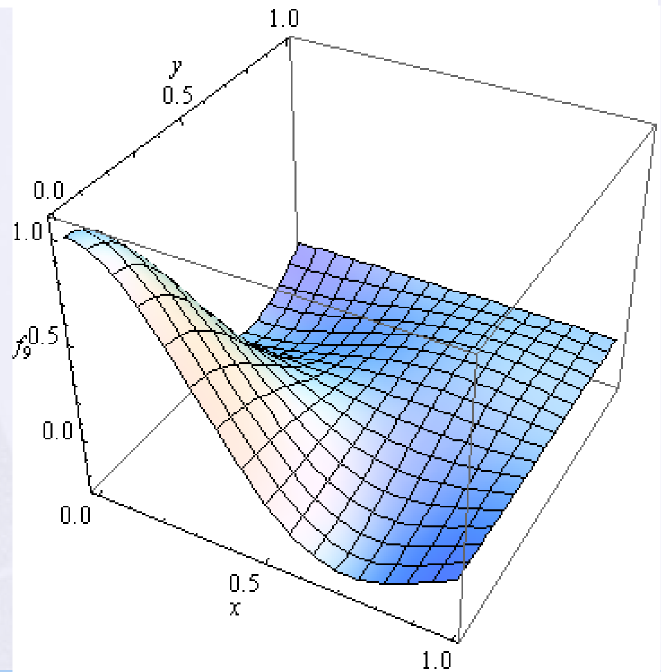
y
0.5
0.0
0.2
0.0
f_8
−0.2
0.0
0.5
x
1.0


1.0
y
0.5
0.0
1.0
f_9
0.5
0.0
0.0
0.5
x
1.0

Error Measures

L_∞ (maximum) error, $\varepsilon_{\max}$, and an L_2 (root-mean-square) error, $\varepsilon_{\mathrm{rms}}$

$$\varepsilon_{\max} = \frac{1}{|f_{\max}|} \max\left\{ \left| f(\mathbf{x}_i) - \hat{f}(\mathbf{x}_i) \right|, i = 1, \ldots, m \right\} \tag{1}$$

$$\varepsilon_{\mathrm{rms}} = \frac{1}{|f_{\max}|} \sqrt{\frac{1}{m} \sum_{i=1}^{m} \left[f(\mathbf{x}_i) - \hat{f}(\mathbf{x}_i) \right]^2} \tag{2}$$

INVERTIBILITY AND POSITIVE DEFINITENESS

Schoenberg and Micchelli

Name	RBF	m
Inverse multiquadric	$(r^2+c^2)^\beta, \quad c>0, \quad \beta<0$	0
Multiquadric	$(-1)^{\lceil\beta\rceil}(r^2+c^2)^\beta, \quad c\geq 0, \quad \beta>0, \quad \beta\notin\mathbb{N}$	$\lceil\beta\rceil$
Gaussian	$\exp(-r^2/c^2), \quad c>0$	0
Polyharmonic spline	$(-1)^{k+1}r^{2k}\ln r, \quad k\in\mathbb{N}$	$k+1$
Shifted logarithmic	$\ln(r^2+c^2), \quad c>0$	1
Shifted spline	$(-1)^{k+1}(r^2+c^2)^k\ln(r^2+c^2), \quad c\geq 0, \quad k\in\mathbb{N}$	$k+1$
Polynomial	$(-1)^{\lceil\beta/2\rceil}r^\beta, \quad \beta>0, \quad \beta\notin 2\mathbb{N}$	$\lceil\beta/2\rceil$

Table 1 Conditionally positive definite radial basis functions of order m. ($\lceil\beta\rceil$ denotes ceiling function, which gives the least integer not smaller than β, and $\mathbb{N}$ is natural number.) Compiled from [64, 65, 69, 74].

NUMERICAL EXPERIMENT

Conclusion

- Missing polynomial augmentation does not seem to be an issue

ERROR ESTIMATE WITH RESPECT TO FILL DISTANCE

Summary by Wendland

Name	RBF	Error Estimate
Inverse multiquadric	$(r^2+c^2)^{\beta}, \quad c>0, \quad \beta<0$	$\exp(-a/h)$
Multiquadric	$(-1)^{\lceil\beta\rceil}(r^2+c^2)^{\beta}, \quad c\geq 0, \quad \beta>0, \quad \beta\notin\mathbb{N}$	$\exp(-a/h)$
Gaussian	$\exp(-r^2/c^2), \quad c>0$	$\exp(-a\log h/h)$
Polyharmonic spline	$(-1)^{k+1}r^{2k}\ln r, \quad k\in\mathbb{N}$	h^{2k}
Polynomial	$(-1)^{\lceil\beta/2\rceil}r^{\beta}, \quad \beta>0, \quad \beta\notin 2\mathbb{N}$	h^{β}

Table 1: Error estimates for various RBF interpolants in terms of fill distance h (following Wendland [95]).

NUMERICAL EXPERIMENT

Polyharmonic Splines

Fill Distance h	RMS Error			
	$r^2 \ln r$	$r^4 \ln r$	$r^6 \ln r$	$r^8 \ln r$
1/4	2.62×10^{-2}	3.12×10^{-2}	4.16×10^{-2}	4.39×10^{-1}
1/8	5.32×10^{-3}	3.90×10^{-3}	3.70×10^{-3}	4.40×10^{-3}
1/16	4.62×10^{-4}	1.36×10^{-4}	5.00×10^{-5}	8.23×10^{-5}
1/32	6.91×10^{-5}	1.11×10^{-5}	2.29×10^{-6}	7.37×10^{-7}
Observed convergence rate	$h^{2.7}$	$h^{3.6}$	$h^{4.4}$	$h^{6.8}$
Theoretical convergence rate	h^2	h^4	h^6	h^8

Table 1: Root mean square error for interpolation of Franke's function 1, using polyharmonic splines. Theoretical convergence rate is based on Wendland [95].

Fill Distance h	Max Error			
	$r^2 \ln r$	$r^4 \ln r$	$r^6 \ln r$	$r^8 \ln r$
1/4	7.70×10^{-2}	7.56×10^{-2}	1.06×10^{-1}	1.46×10^{0}
1/8	3.98×10^{-2}	2.90×10^{-2}	2.45×10^{-2}	2.10×10^{-2}
1/16	4.66×10^{-3}	1.40×10^{-3}	3.02×10^{-4}	6.26×10^{-4}
1/32	1.56×10^{-3}	2.54×10^{-4}	2.29×10^{-5}	8.10×10^{-6}
Observed convergence rate	$h^{1.6}$	$h^{2.5}$	$h^{3.7}$	$h^{6.3}$
Theoretical convergence rate	h^2	h^4	h^6	h^8

Table 2: Maximum error for interpolation of Franke's function 1, using polyharmonic splines. Theoretical convergence rate is based on Wendland [95].

Gaussian and IMQ

Fill Distance h	f_8		f_9	
	GA	IMQ	GA	IMQ
1/5	1.08×10^{-2}	7.94×10^{-2}	1.82×10^{-3}	6.21×10^{-3}
1/10	2.45×10^{-7}	1.34×10^{-5}	2.47×10^{-8}	2.34×10^{-7}
1/20	1.32×10^{-18}	4.87×10^{-17}	7.89×10^{-20}	5.90×10^{-19}
1/30	8.52×10^{-31}	1.16×10^{-27}	5.29×10^{-32}	1.46×10^{-29}
Observed convergence rate	$\lambda^{1/h^{1.3\sim1.4}}$	$\lambda^{1/h^{1.2\sim1.7}}$	$\lambda^{1/h^{1.2\sim1.3}}$	$\lambda^{1/h^{1.1\sim1.5}}$

Table 1: Root mean square error of interpolation of two functions using inverse multiquadric (IMQ) and Gaussian (GA) for various fill distances. $c=1.5$ and 6.0 are respectively used for GA and IMQ.

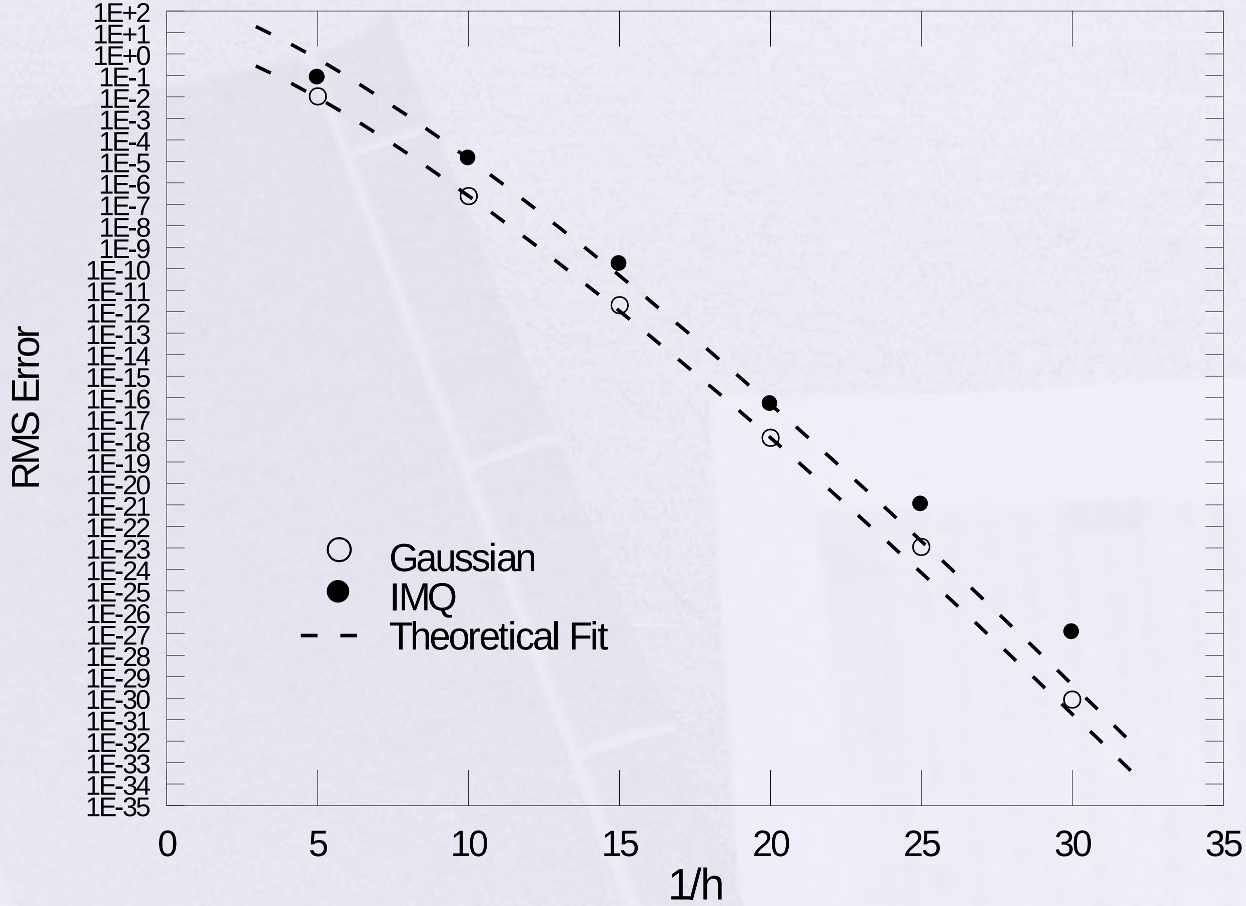


Figure 1: Root mean square error for interpolation of f_8 using Gaussian and inverse multiquadric. The dashed lines are given by $\varepsilon = 2.65\,h^{0.703/h}$ for Gaussian, and $\varepsilon = 185\,h^{0.714/h}$ for IMQ.

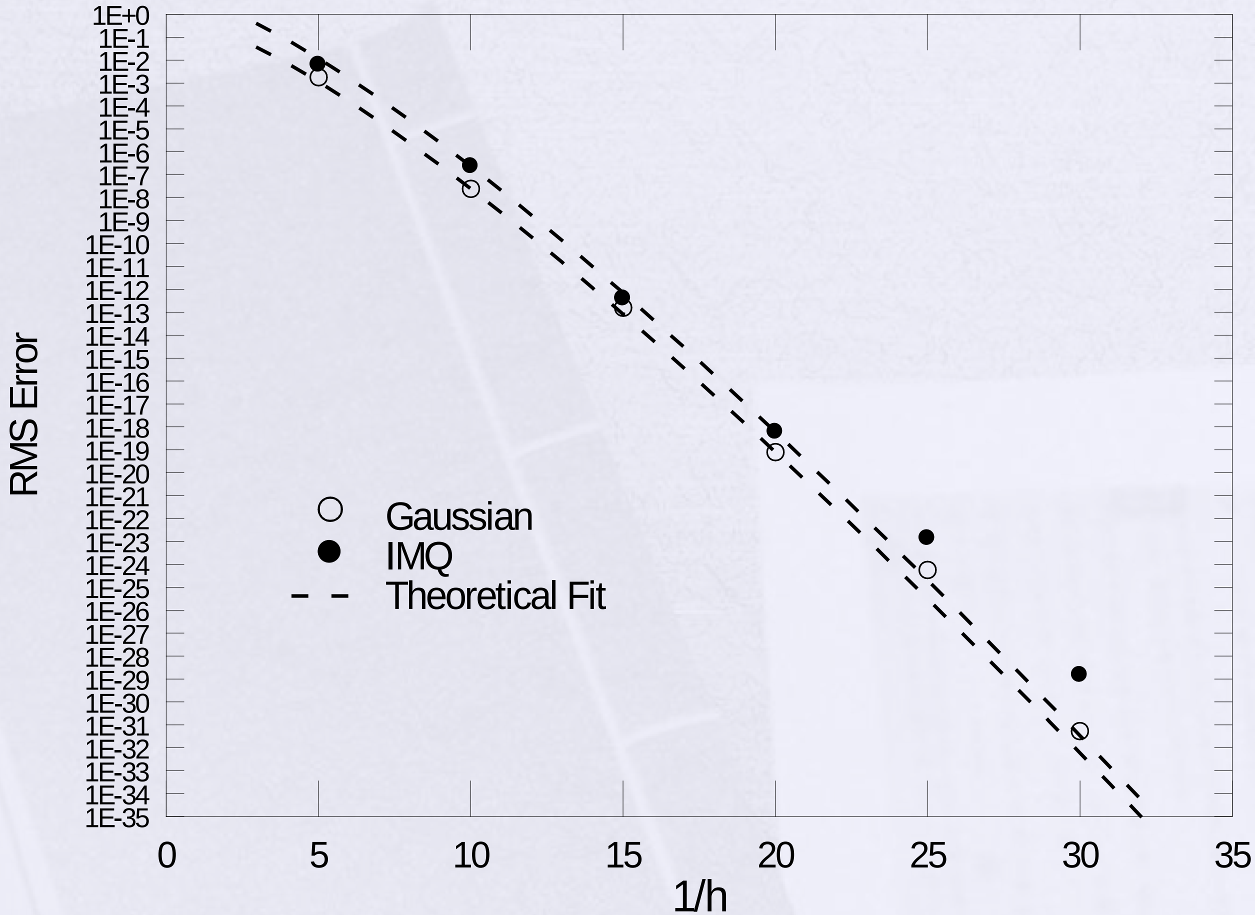


Figure 1: Root mean square error for interpolation of f_9 using Gaussian and inverse multiquadric. The dashed lines are given by $\varepsilon = 0.37\, h^{0.718/h}$ for Gaussian, and $\varepsilon = 4.06\, h^{0.724/h}$ for IMQ.

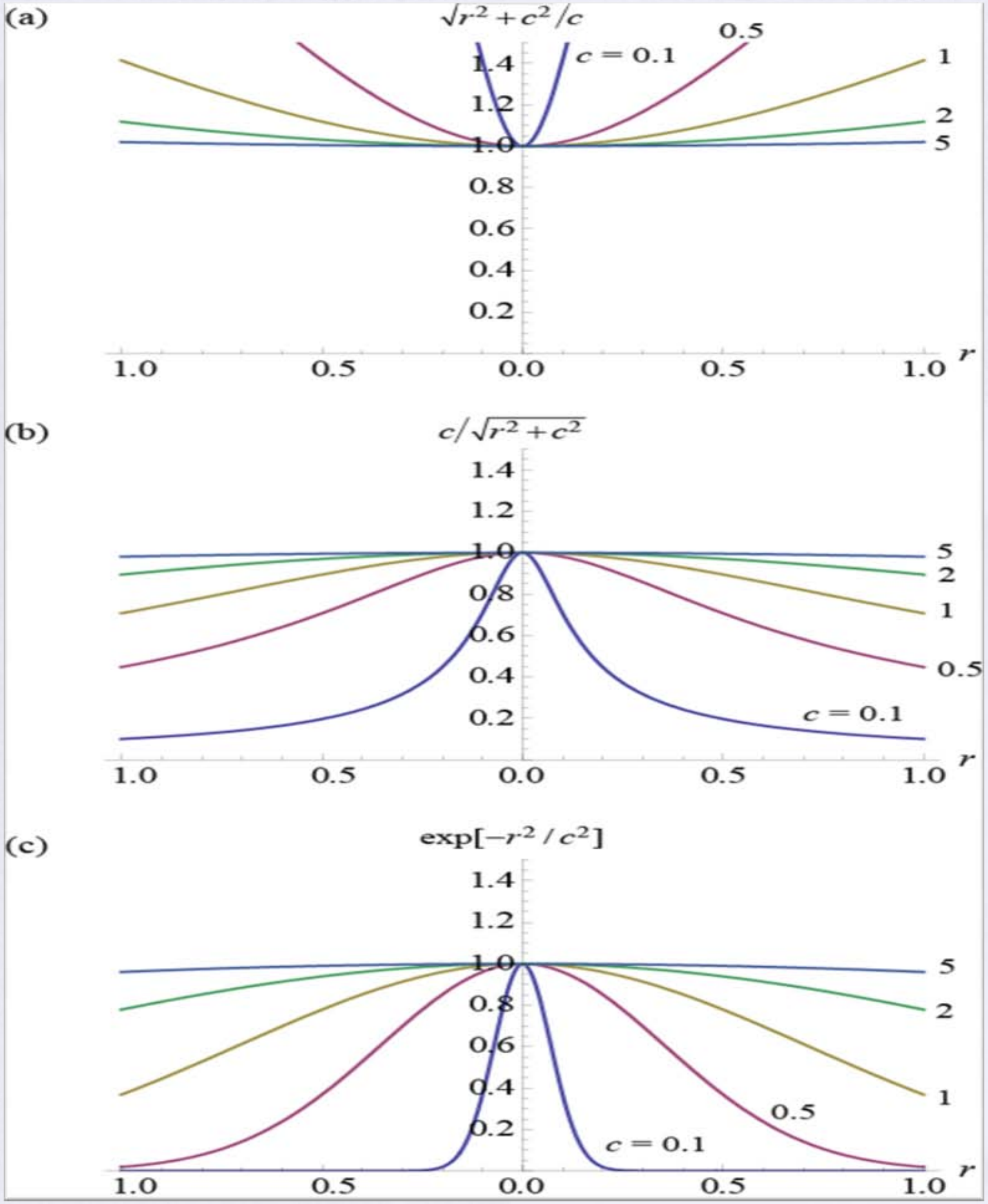
Summary of Error Estimate

$$(-1)^{k+1} r^{2k} \ln r, \quad \varepsilon \sim O(h^{2k})$$

$$(r^2 + c^2)^{-1/2}, \quad \varepsilon \sim O(h^{1/h})$$

INFINITELY FLAT RBF

Flattening of the basis function by adjusting the shape factor: (a) multiquadric (normalized), (b) inverse multiquadric (normalized), and (c) Gaussian.



Flatness

- As the basis function becomes flatter, the interpolant becomes more accurate.
- The matrix becomes more ill-conditioned, and finite precision numerical solution of the matrix fails.
- But the matrix remains positive definite and is in theory solvable.

Theoretical Limit as $\varepsilon = (1/c) \rightarrow 0$

- Baxter 1992; Driscoll and Fornberg 2002; Fornberg et al. 2004; Larsson and Fornberg 2005; Schaback 2005:
- MQ behaves like polynomials, particularly in 1-D, it becomes Lagrangian polynomial interpolation.

NUMERICAL EXPERIMENT

Interpolation by IMQ in 2D with Uniform Grid

In this first example, we use IMQ to interpolate the function $u = \sin(2\pi x) + \cos(2\pi y)$. A 21×21 uniform grid is laid over the unit square domain, to give a mesh size $h = 1/20$. The interpolation is performed using a whole range

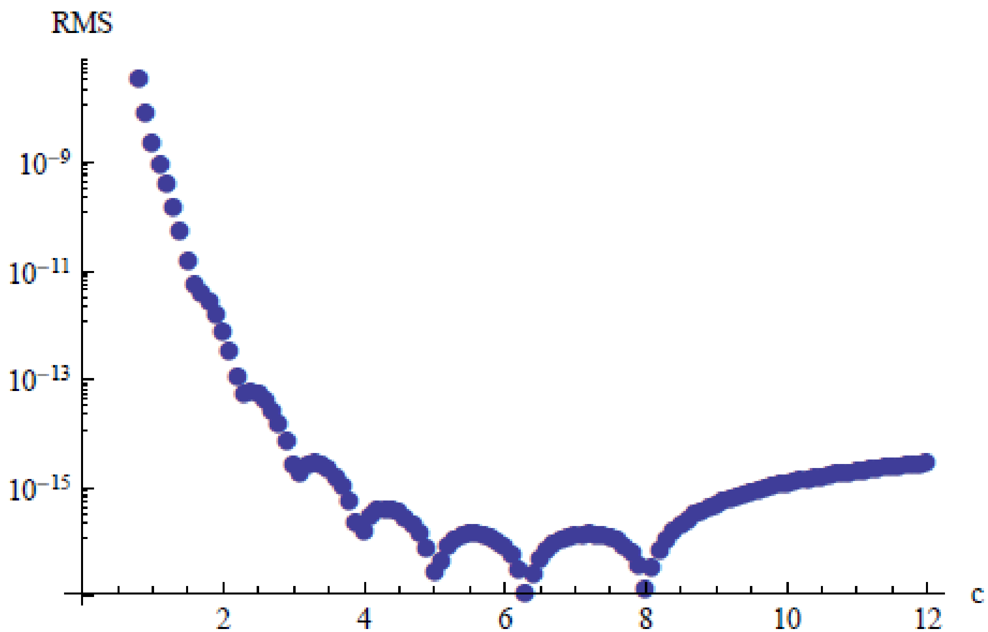


Figure 2. RMS error $\varepsilon_{\mathrm{RMS}}(s, u)$ for interpolating $u = \sin(2\pi x) + \cos(2\pi y)$ using IMQ: mesh size $h = 1/20$, in smaller c range.

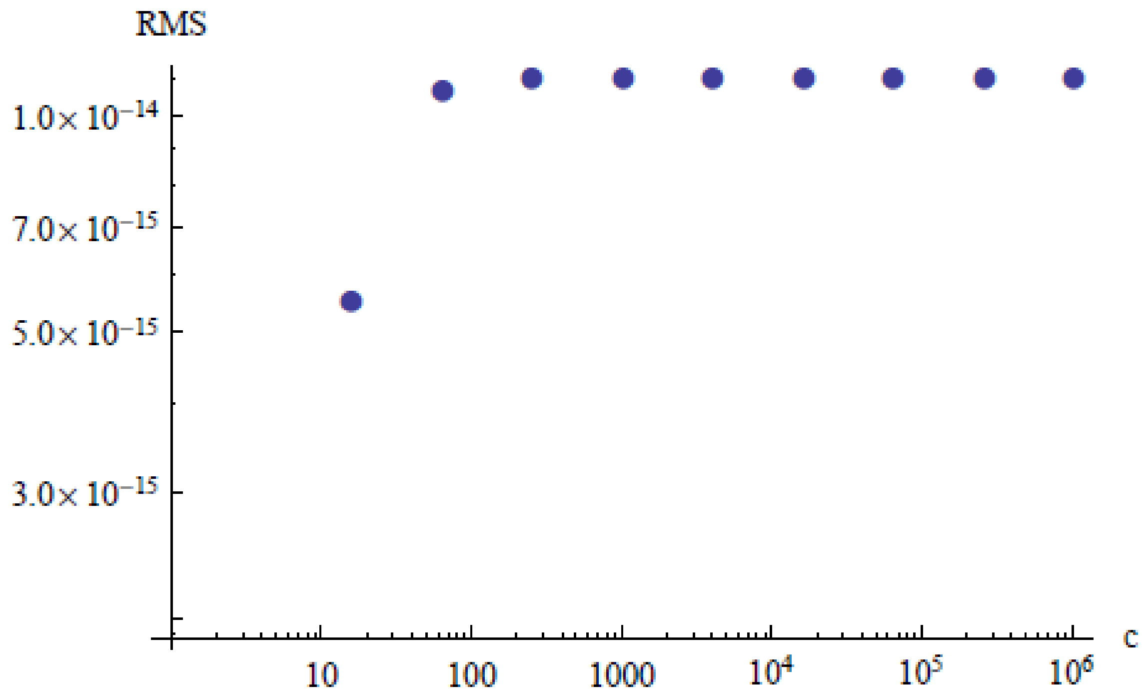


Figure 1. RMS error $\varepsilon_{\mathrm{RMS}}(s,u)$ for interpolating $u=\sin(2\pi x)+\cos(2\pi y)$ using IMQ: mesh size $h=1/20$, in large c range.

As a confirmation of polynomial limit, we have tested a number of polynomial functions, with only one example given here as an illustration. For the case $u = x^2y$, we use a uniform grid with $h = 1/10$ for interpolation. The resultant

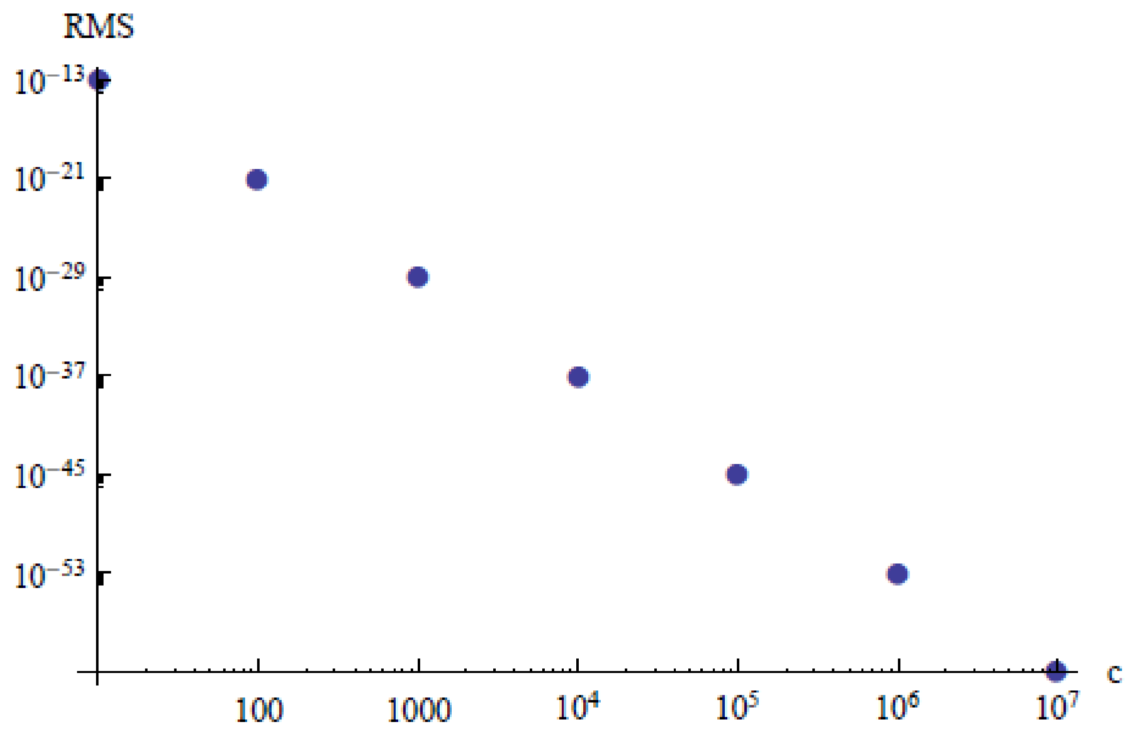


Figure 3. RMS error $\varepsilon_{\mathrm{RMS}}(s, u)$ for interpolating $u = x^2y$ using IMQ: mesh size $h = 1/10$, in large c range.

We now use IMQ to interpolate $u = \sin(2\pi x)\cos(2\pi y)$ over the unit square.

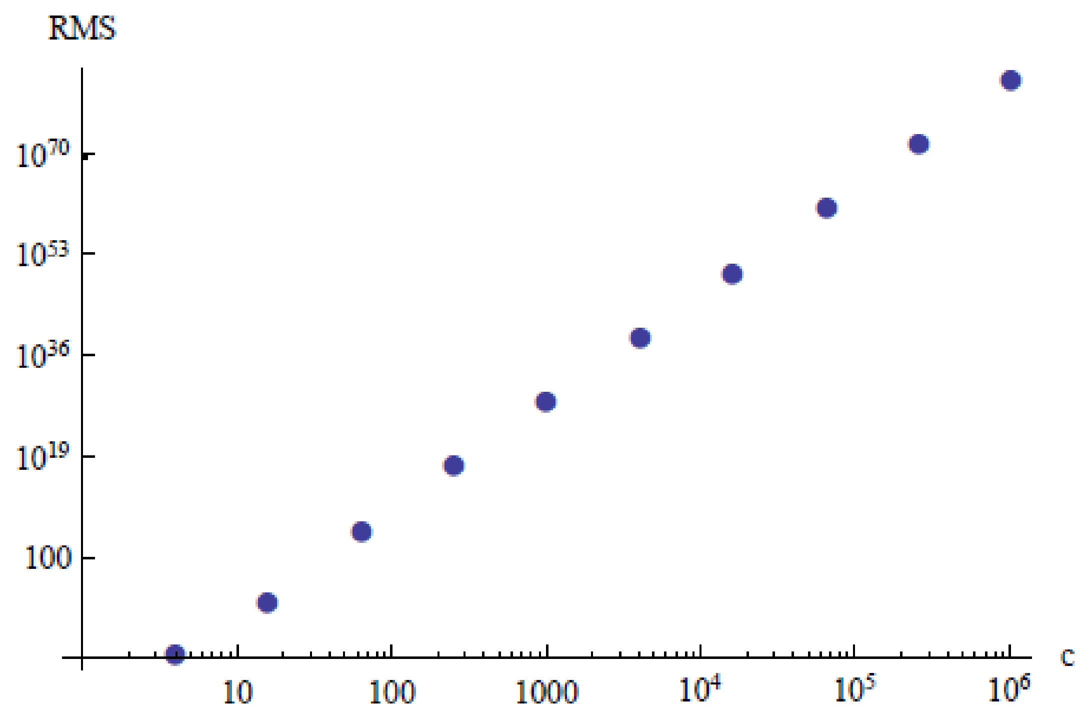


Figure 5. RMS error $\varepsilon_{\mathrm{RMS}}(s, u)$ for interpolating $u = \sin(2\pi x)\cos(2\pi y)$ using IMQ: mesh size $h = 1/20$, in large c range.

Interpolation by GA with Uniform Grid

For the function $u = \sin(2\pi x)\cos(2\pi y)$,

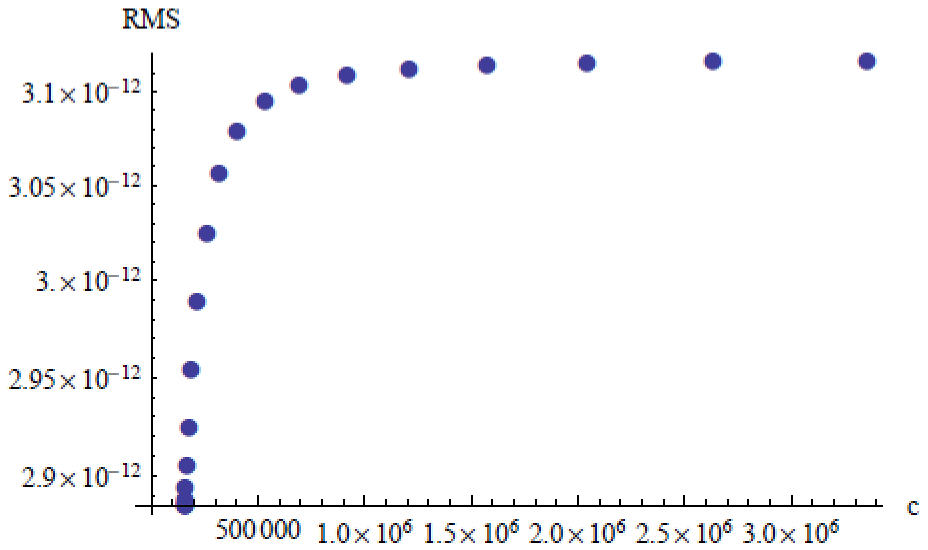


Figure 7. RMS error $\varepsilon_{\mathrm{RMS}}(s,u)$ for solution of PDE with exact solution $u(x,y) = \sin(2\pi x) + \cos(2\pi y)$ using IMQ: mesh size $h = 1/20$, in large c range.

Conclusion: Huang, et al (2010)

- For interpolation in *one-dimensional* space using a class of infinitely smooth basis functions that can be expanded into a power series (this class includes GA, MQ, IMQ, etc.), the interpolant converges to a polynomial limit as the basis functions are continuously flattened by taking $\delta = (1/c) \to 0$ (see [24]) . The asymptotic error of the interpolation as $\delta \to 0$ is $\varepsilon \sim O(\delta^2)$.

- For interpolation in *two-dimensional* space using IMQ on a *uniform* grid, the IMQ interpolant can diverge or converge, as $c \to \infty$, depending on the function interpolated. Based on observation, the interpolant converges for essentially one-dimensional functions (such as $\sin(2\pi x) + \cos(2\pi y)$) and bivariate polynomials (such as $x^2 y$). In the latter case, the error converges to zero. Divergent behavior is observed for all other functions.

- On a *random* grid, the IMQ interpolant converges for all functions as $c \to \infty$.
- For interpolation in *two-dimensional* space, GA interpolant always converges as $c \to \infty$, whether the grid is uniform or random [33].

- For two-dimensional cases, whether the interpolant converges or diverges, an optimal c exists at a finite value, with the exception of the polynomial function (in that case, $\varepsilon \to 0$ as $c \to \infty$).

ERROR ESTIMATE WITH RESPECT TO SHAPE PARAMETER

Madych (1972)

Madych's theoretical analysis in 1992 [75] was the first, and until recently the only, error bound that contains the shape parameter c. Madych's results are presented for two different classes of functions, B_σ and E_σ:

$$B_\sigma = \left\{ f \in L^2(\mathbb{R}^n) : \tilde{f}(\xi) = 0 \text{ if } \|\xi\| > \sigma \right\} \tag{43}$$

$$E_\sigma = \left\{ f \in L^2(\mathbb{R}^n) : \|\tilde{f}\|_{E_\sigma} < \infty \right\} \tag{44}$$

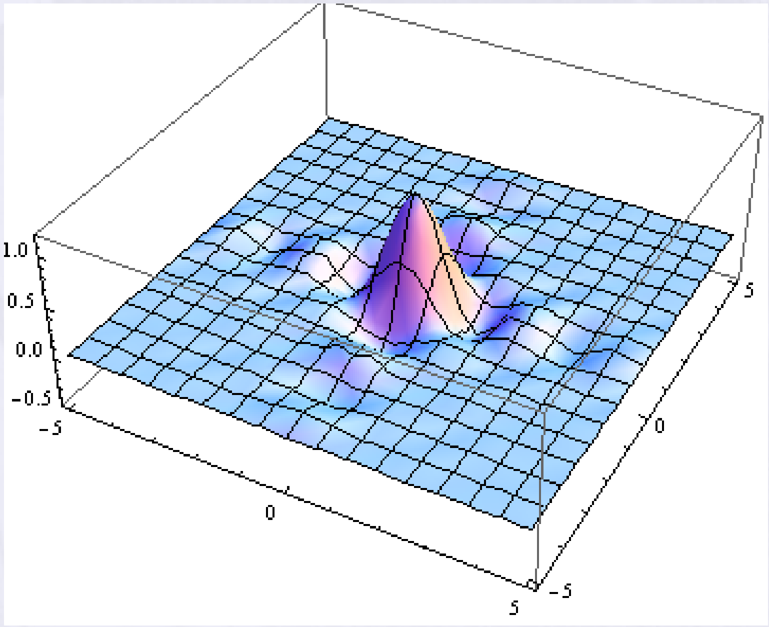
where σ is a positive constant,

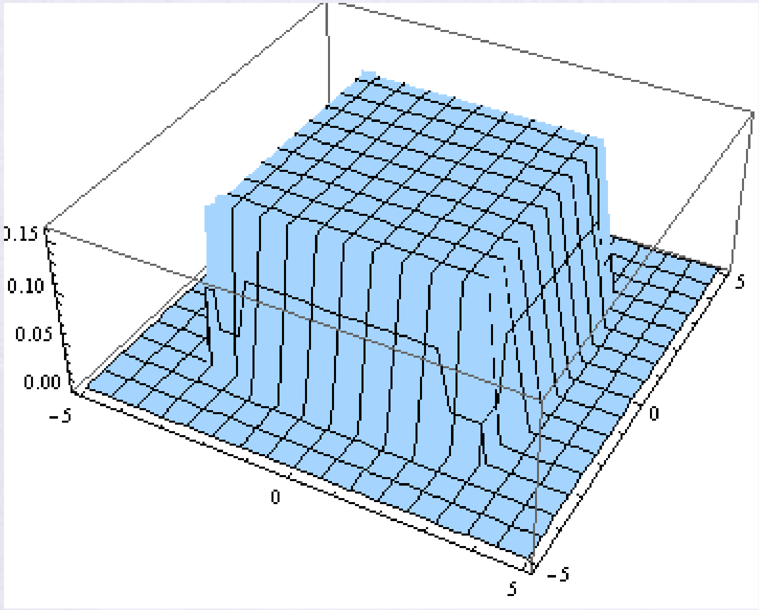
$$\tilde{f}(\xi) = \int_{\mathbb{R}^n} f(\mathbf{x})\, e^{-i(\mathbf{x}\xi)}\, d\mathbf{x} \tag{45}$$

is the multivariate Fourier transform of function $f(\mathbf{x})$, and

$$\|\tilde{f}\|_{E_\sigma}^2 = \int_{\mathbb{R}^n} \left|\tilde{f}(\xi)\right|^2 e^{|\xi|^2/\sigma}\, d\xi \tag{46}$$

A Band Limited Function





$$\frac{\sin(\pi x)}{\pi x}\frac{\sin(\pi y)}{\pi y}$$

Its Fourier Transform

For a class of interpolators that include GA, MQ and IMQ, Madych provided the following error estimates: for $f \in B_\sigma$,

$$\varepsilon \sim O\left(e^{ac}\lambda^{c/h}\right), \quad \text{for} \quad 0<\lambda<1 \quad \text{and} \quad a>0 \qquad (47)$$

and for $f \in E_\sigma$,

$$\varepsilon \sim O\left(e^{ac^2}\lambda^{c/h}\right), \quad \text{for} \quad 0<\lambda<1 \quad \text{and} \quad a>0 \qquad (48)$$

We observe that these error estimates are made of the product of two competing terms as *c* becomes large—one part grows exponentially, and the other decays exponentially.

Luh (2010)

The only other theoretical error estimate that explores the role of the shape parameter c is provided by Luh [67-72]. The error estimates are generally expressed as

$$\varepsilon \sim O\left(MN(c)\lambda^{1/h}\right), \quad \text{for} \quad 0<\lambda<1 \tag{49}$$

where $MN(c)$ is the part of the error estimate that is dependent on c. Methods are provided for the estimate of λ, and the optimal value of c, which will be further discussed in Section 11.

Luh [71] derived, based the node laid on the vertices of a uniform n-simplex in $\mathbb{R}^n$, the following estimates for the MQ family interpolating $f \in B_\sigma$

$$MN(c) = e^{c\sigma/2} c^{(1+\beta-n-4\ell)/4} \quad \text{for} \quad 1+\beta-n-4\ell<0 \tag{53}$$

where β is as defined in Table 1, and $\beta=-1/2$ for IMQ, $n=2$ for the two-dimensional functions interpolated, $\ell \approx 1/h$, and σ is the range of the band limited function in Fourier transform space, as defined in (43). For the function (41), $\sigma = 2\pi$. We can easily differentiate (53) to obtain the optimal c

NUMERICAL EXPERIMENT

Empirical Error Estimate

- IMQ

$$\varepsilon \sim O\left(e^{ac^{3/2}} \lambda^{c^{1/2}/h}\right), \quad \text{for} \quad 0<\lambda<1 \quad \text{and} \quad a>0$$

- Gaussian

$$\varepsilon \sim O\left(e^{ac^{4}} \lambda^{c/h}\right), \quad \text{for} \quad 0<\lambda<1 \quad \text{and} \quad a>0$$

OPTIMAL SHAPE PARAMETER

f_1				f_5			
c	Gauss	c	IMQ	c	Gauss	c	IMQ
0.1	1.01E-02	0.1	2.28E-03	0.1	3.13E-04	0.1	9.93E-04
0.2	2.25E-03	0.2	1.36E-03	0.2	9.89E-07	0.5	2.00E-06
1.0	9.47E-03	1.0	4.47E-03	1.0	3.53E-03	1.0	1.74E-04
f_2				f_6			
c	Gauss	c	IMQ	c	Gauss	c	IMQ
0.1	2.35E-02	0.1	6.83E-03	0.1	8.97E-03	0.1	5.99E-03
0.2	4.11E-03	0.4	2.68E-03	10	1.95E-06	1.3	1.87E-06
1.0	8.22E-02	1.0	5.08E-02	100	1.94E-06	2.0	9.82E-06
f_3				f_8			
c	Gauss	c	IMQ	c	Gauss	c	IMQ
0.1	1.59E-02	0.1	3.90E-03	0.1	5.94E-03	0.1	2.90E-03
0.3	1.58E-04	0.6	1.12E-04	1.2	3.49E-08	3.4	1.52E-07
1.0	1.16E-03	1.0	2.57E-04	2.0	7.14E-07	5.0	2.75E-06
f_4				f_9			
c	Gauss	c	IMQ	c	Gauss	c	IMQ
0.1	3.45E-03	0.1	1.87E-03	0.1	1.16E-02	0.1	3.31E-03
0.4	8.11E-12	1.5	1.26E-08	1.0	1.27E-09	4.1	8.21E-09
1.0	1.96E-06	2.0	5.99E-08	2.0	1.00E-07	10	3.71E-04

Table 1: Root mean square error for interpolating functions f_1 through f_9, using Gaussian and IMQ, with mesh size $h = 0.1$, and various c values.

Shape Factor

- Madych (1992): For the interpolation of a class of "essentially analytic functions", which are "band limited", using a class of basis functions that include the multiquadric, Gaussian, …, he proved

$$\varepsilon = O\left(e^{ac}\lambda^{c/h}\right); \quad 0<\lambda<1, \quad a>0$$

- This means, as $c \to \infty, \quad \varepsilon \to 0$

- Madych also stated that for a “non-band-limited” function,

$$\varepsilon = O\left(e^{ac^2}\lambda^{c/h}\right); \quad 0<\lambda<1, \quad a>0$$

- In this case, there exist a $c_{opt} = -\dfrac{\ln\lambda}{2ah}$ where $\varepsilon = \varepsilon_{\min}$
- If we can use the c_{opt} then $\varepsilon \sim O(\lambda^{1/h^2})$

Luh (2011)

Luh [71] derived, based the node laid on the vertices of a uniform n-simplex in $\mathbb{R}^n$, the following estimates for the MQ family interpolating $f \in B_\sigma$

$$MN(c) = e^{c\sigma/2} c^{(1+\beta-n-4\ell)/4} \quad \text{for} \quad 1+\beta-n-4\ell<0 \tag{53}$$

where β is as defined in Table 1, and $\beta=-1/2$ for IMQ, $n=2$ for the two-dimensional functions interpolated, $\ell \approx 1/h$, and σ is the range of the band limited function in Fourier transform space, as defined in (43). For the function (41), $\sigma = 2\pi$. We can easily differentiate (53) to obtain the optimal c value as

$$c_{\text{opt}} \approx \frac{-1-\beta+n+4\ell}{2\sigma} \tag{54}$$

For sufficiently small fill distance h, we can express $c_{\text{opt}} \approx 2/\sigma h$.

NUMERICAL EXPERIMENT

Empirical Optimal Shape Parameter

- IMQ

$$\varepsilon \sim O\left(e^{ac^{3/2}} \lambda^{c^{1/2}/h}\right), \quad \text{for} \quad 0 < \lambda < 1 \quad \text{and} \quad a > 0$$

$$c_{\text{opt}} \sim O\left(\frac{-\ln\lambda}{3ah}\right)$$

- Gaussian

$$\varepsilon \sim O\left(e^{ac^{4}} \lambda^{c/h}\right), \quad \text{for} \quad 0 < \lambda < 1 \quad \text{and} \quad a > 0$$

$$c_{\text{opt}} \sim O\left(\frac{(-\ln\lambda)^{1/3}}{2^{2/3} a^{1/3} h^{1/3}}\right)$$

$1/h$	IMQ				GA			
	f_8		f_9		f_8		f_9	
	c_{opt}	ε_{rms}	c_{opt}	ε_{rms}	c_{opt}	ε_{rms}	c_{opt}	ε_{rms}
4	1.5	6.53E-03	1.6	1.17E-03	0.7	3.16E-03	0.8	2.20E-04
8	3.0	4.96E-06	2.5	9.66E-07	1.1	2.85E-06	1.1	2.25E-07
16	4.7	3.42E-13	5.5	8.00E-15	1.4	3.01E-14	1.4	6.00E-17
32	8.1	1.83E-30	8.9	4.74E-33	1.8	1.09E-33	1.8	5.57E-36

Table 9: Optimal c and the corresponding error for interpolating two functions by IMQ and GA.

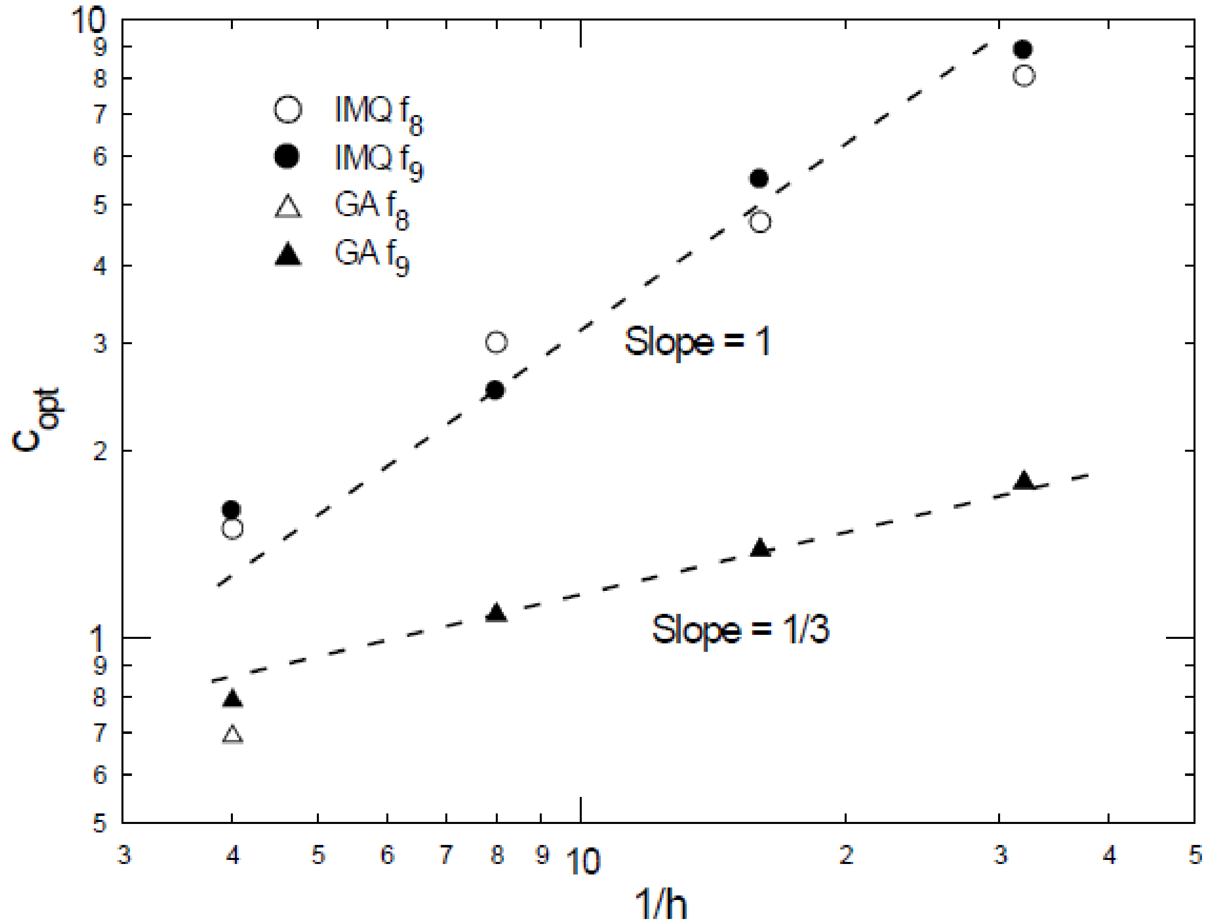


Figure 6: Plot of optimal c versus $1/h$ for IMQ and GA interpolating f_8 and f_9.

Luh (2011)

We should also mention that the formulas provided by Luh [70, 71] also seem to work well. For example, for MQ interpolating the band limited function f_9, equation (54) predicts the optimal c values as 1.4, 2.7, 5.2 and 10.3, respectively for $1/h = 4, 8, 16, 32$. These can be compared to the 1.6, 2.5, 5.5 and 8.9 c_{opt} values reported in Table 9.

Error Estimate with Fill Distance Using Optimal Shape Parameter

- IMQ

$$\varepsilon_{\min} \sim O\left(\exp\left(-\frac{2(-\ln\lambda)^{3/2}}{3^{3/2}a^{1/2}h^{3/2}}\right)\right)$$

- Gaussian

$$\varepsilon_{\min} \sim O\left(\exp\left(-\frac{3(-\ln\lambda)^{4/3}}{2^{8/3}a^{1/3}h^{4/3}}\right)\right)$$

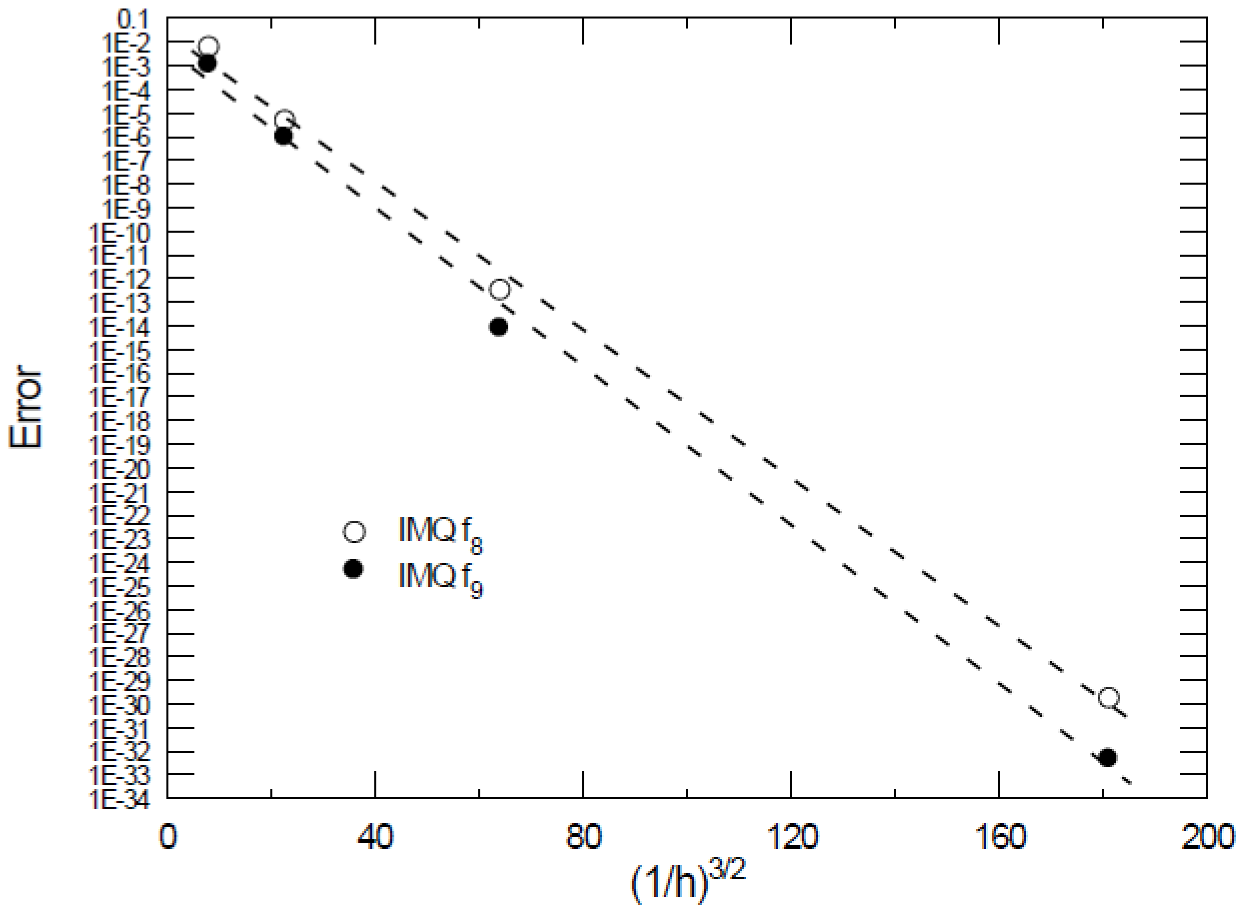


Figure 7: Plot of minimum error versus $(1/h)^{3/2}$ for IMQ interpolating f_8 and f_9.

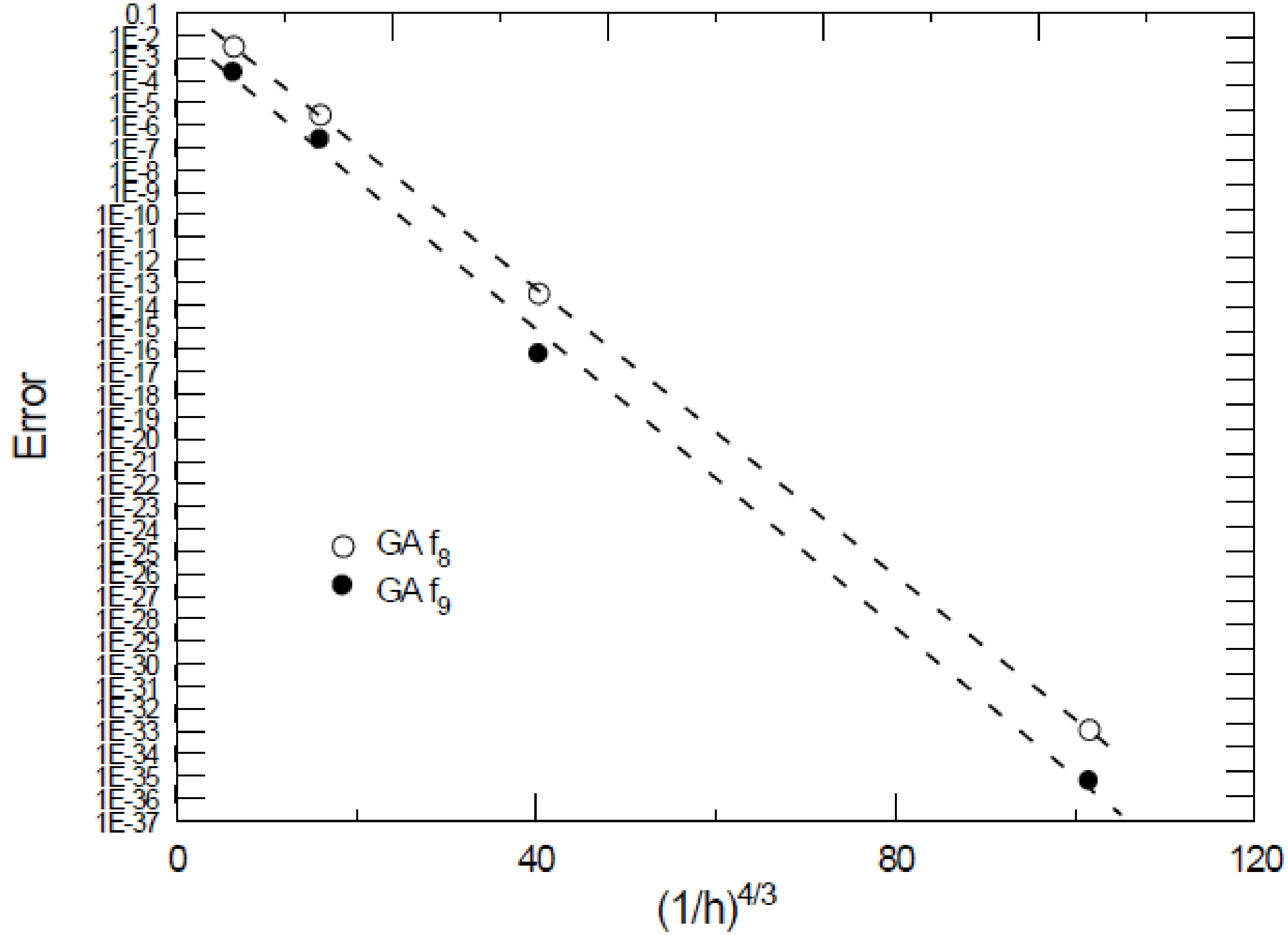


Figure 8: Plot of minimum error versus $(1/h)^{3/2}$ for IMQ interpolating f_8 and f_9.

CONDITION NUMBER AND EFFECTIVE CONDITION NUMBER

Upper Bound for Condition Number

Ball [1] appears to be the first to investigate condition number associated with radial basis functions. For $\varphi = r$, he provided the following upper bound for condition number

$$\kappa \leq \left(\frac{D}{2q}\right)^{d+1} \tag{1}$$

where $q = (1/2)\min_{j \neq k}\left\|\mathbf{x}_j - \mathbf{x}_k\right\|$ is half the smallest separating distance between data points, $D = \max_{j \neq k}\left\|\mathbf{x}_j - \mathbf{x}_k\right\|$ is the diameter of the data set (or, the size of the domain, assuming that the domain is well covered by the data set), and d is the dimension of the data set (or the interpolated domain).

Norwich and Ward

d	r	$\sqrt{1+r^2}$	$\ln(1+r^2)$
2	$7(D/h)^3$	$48(D^2/h^4)\sqrt{1+D^2}\exp(24/h^2)$	$(D^2/h^2)\log(1+D^2)/K_0(24/h^2)$
3	$9(D/h)^4$	$68(D^3/h^5)\sqrt{1+D^2}\exp(32/h^2)$	$2(D^3/h^3)\log(1+D^2)/K_0(32/h^2)$

Table 1: Upper bound condition number for three radial basis functions, corresponding to a uniform grid.

Based on the work of Norwich and Ward [71], Ball, *et al*. [2] presented an estimate for inverse multiquadric $\varphi = 1/\sqrt{1+r^2}$ upper bound for condition number as

$$\kappa \leq C \frac{D^d}{h^d \sqrt{1+D^2}} \exp\left(\frac{2d}{h}\right) \tag{1}$$

where d is the dimension.

For multiquadric $\varphi = \sqrt{c^2 + r^2}$, Buhman [11] reported that the following upper bound

$$\kappa \leq C \sqrt{c^2 + D^2} \frac{D^d}{h^{d+1}} \exp\left(\frac{8dc}{h}\right) \tag{1}$$

NUMERICAL EXPERIMENT

h	c	Condition Number		
		MQ	IMQ	Gaussian
0.2	1.0	3.41×10^{9}	1.83×10^{8}	1.15×10^{13}
0.1	1.0	5.21×10^{18}	1.39×10^{17}	2.26×10^{33}
0.05	1.0	5.47×10^{36}	7.26×10^{34}	1.17×10^{80}
0.04	1.0	4.76×10^{45}	5.04×10^{43}	1.86×10^{105}
0.033	1.0	3.89×10^{54}	3.43×10^{52}	2.23×10^{131}

Table 1: Condition numbers for multiquadric, inverse multiquadric, and Gaussian interpolation on a 1×1 square, with $c=1$.

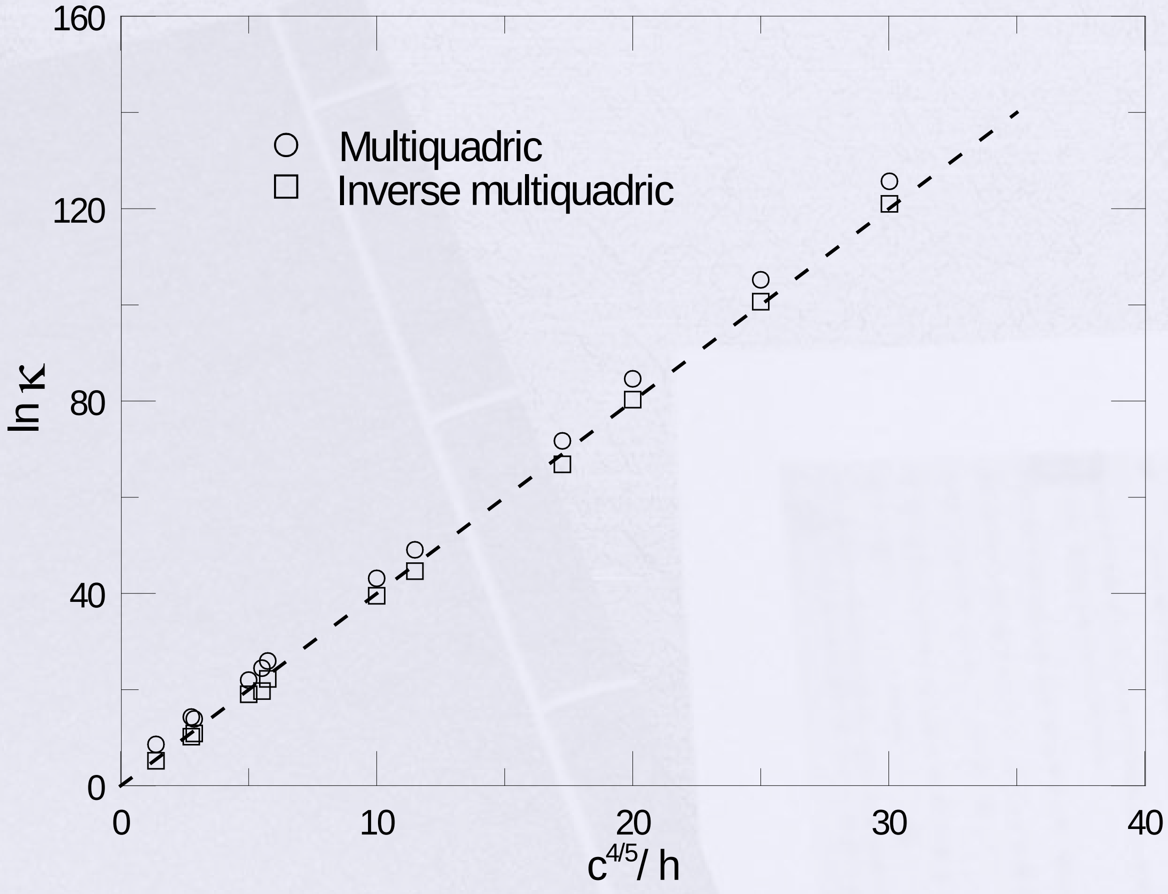


Figure 1: Log condition number $\ln \kappa$ versus $c^{4/5}/h$ for multiquadric and inverse multiquadric, with a range of c and h values, for $c \leq 1$. Symbols: computed result; dashed line: slope of 4.

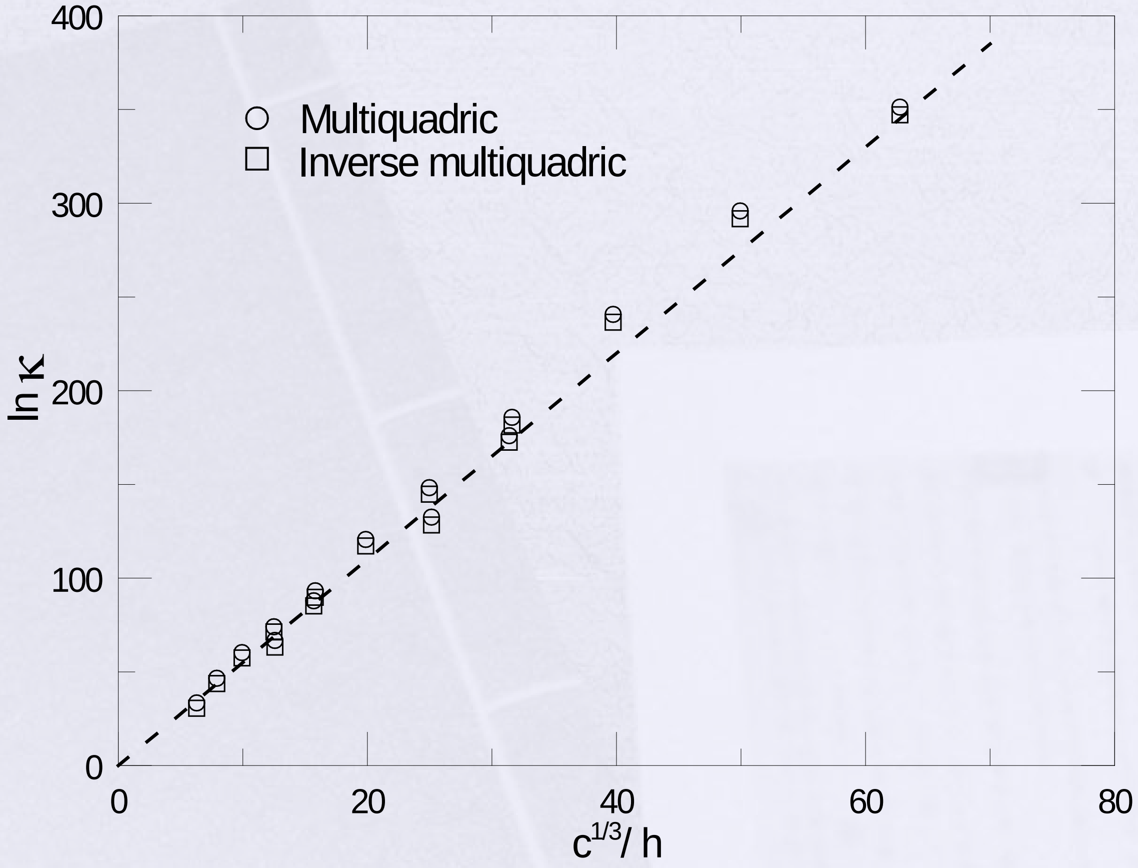


Figure 1: Log condition number $\ln\kappa$ versus $c^{1/3}/h$ for multiquadric and inverse multiquadric, with a range of c and h values, for $c > 1$. Symbols: computed result; dashed line: slope of 5.5.

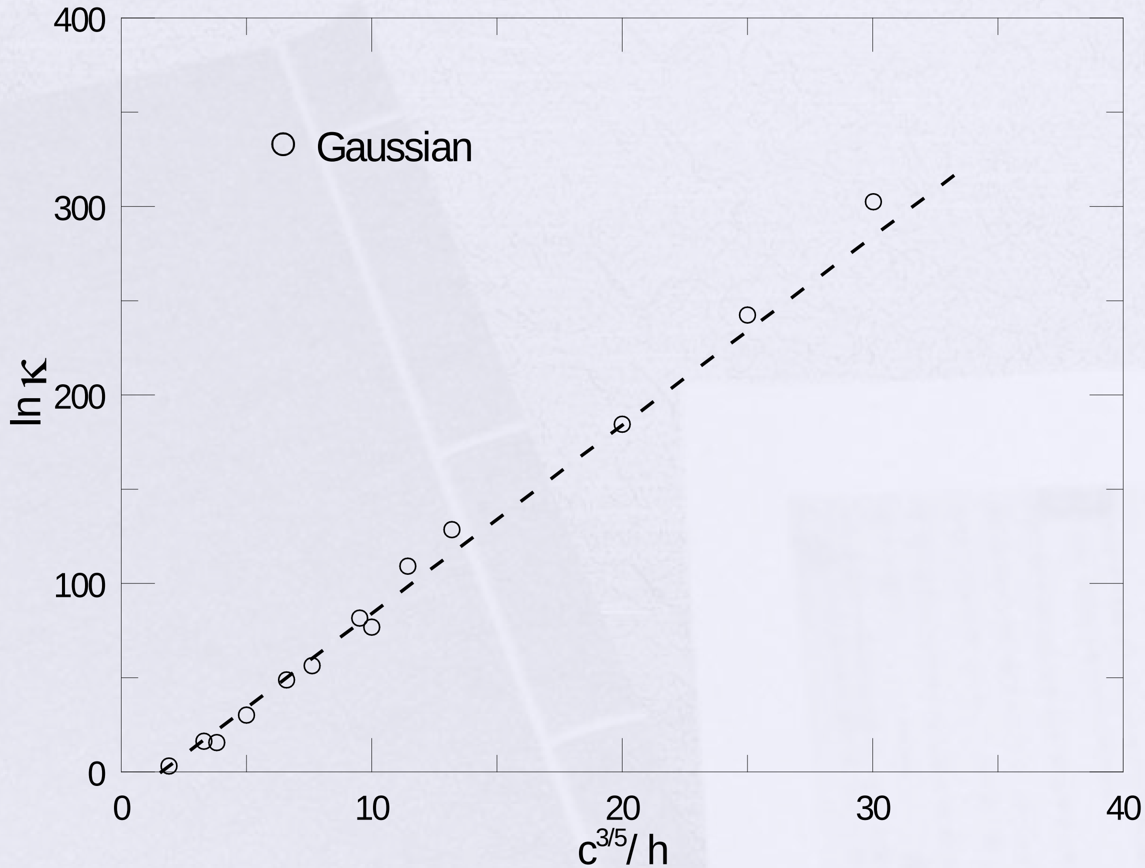


Figure 1: Log condition number $\ln\kappa$ versus $c^{3/5}/h$ for Gaussian, with a range of c and h values, for $c \leq 1$. Symbol: computed result; dashed line: slope of 10.

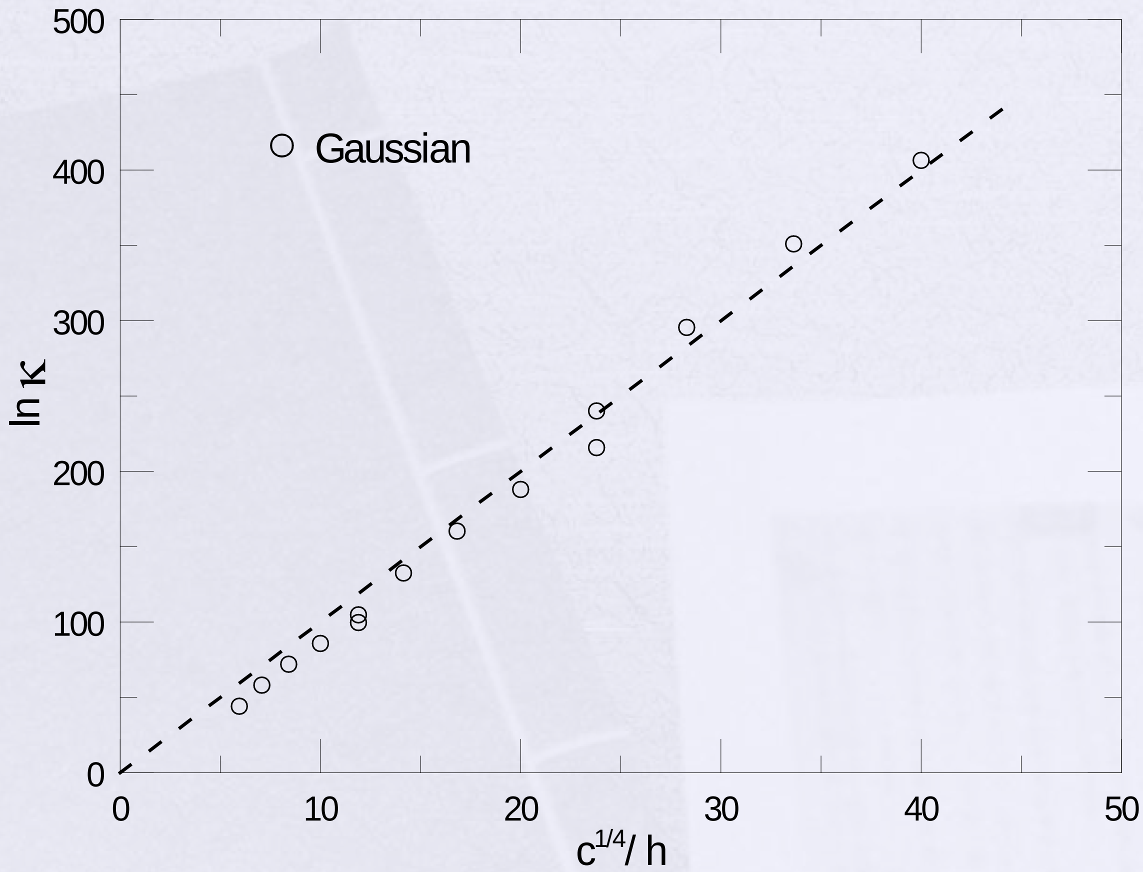


Figure 1: Log condition number $\ln\kappa$ versus $c^{1/4}/h$ for Gaussian, with a range of c and h values, for $c > 1$. Symbol: computed result; dashed line: slope of 10.

Condition Number Based on Observation

Based on the observed fits, we present the following estimate of condition number on a uniform grid, for both multiquadric and inverse multiquadric

$$\kappa \sim O\left(\exp\left(\frac{4\,c^{4/5}}{h}\right)\right); \quad c \le 1$$
$$\kappa \sim O\left(\exp\left(\frac{5.5\,c^{1/3}}{h}\right)\right); \quad c > 1 \qquad (1)$$

Based on the data, the following estimate of condition number for Gaussian is given

$$\kappa \sim O\left(\exp\left(\frac{10\,c^{3/5}}{h}\right)\right); \quad c \le 1$$
$$\kappa \sim O\left(\exp\left(\frac{10\,c^{1/4}}{h}\right)\right); \quad c > 1 \qquad (1)$$

Effective Condition Number

The traditional condition number as defined by Wilkinson [97, 98] is the maximum ratio of the relative error in $\{\mathbf{X}\}$ divided by the relative error in $\{\mathbf{b}\}$, and is given by

$$\kappa = \|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\| = \left|\frac{\sigma_1}{\sigma_N}\right| \qquad (1)$$

The effective condition number that takes into account the right hand side vector, according to Rice [67], Banoczi *et al* [3], and Christiansen and Saranen [18], is

$$\kappa_{\text{eff}} = \frac{\|\mathbf{b}\|}{\|\mathbf{X}\|}\|\mathbf{A}^{-1}\| \quad (1)$$

ROUND-OFF ERROR AND INSTABILITY

Approximation Error and Round-Off Error

Approximation error $\left\| f(\mathbf{x}) - \hat{f}(\mathbf{x}) \right\|$

Round-off error $\left\| \hat{f}(\mathbf{x}) - \overline{f}(\mathbf{x}) \right\|$.

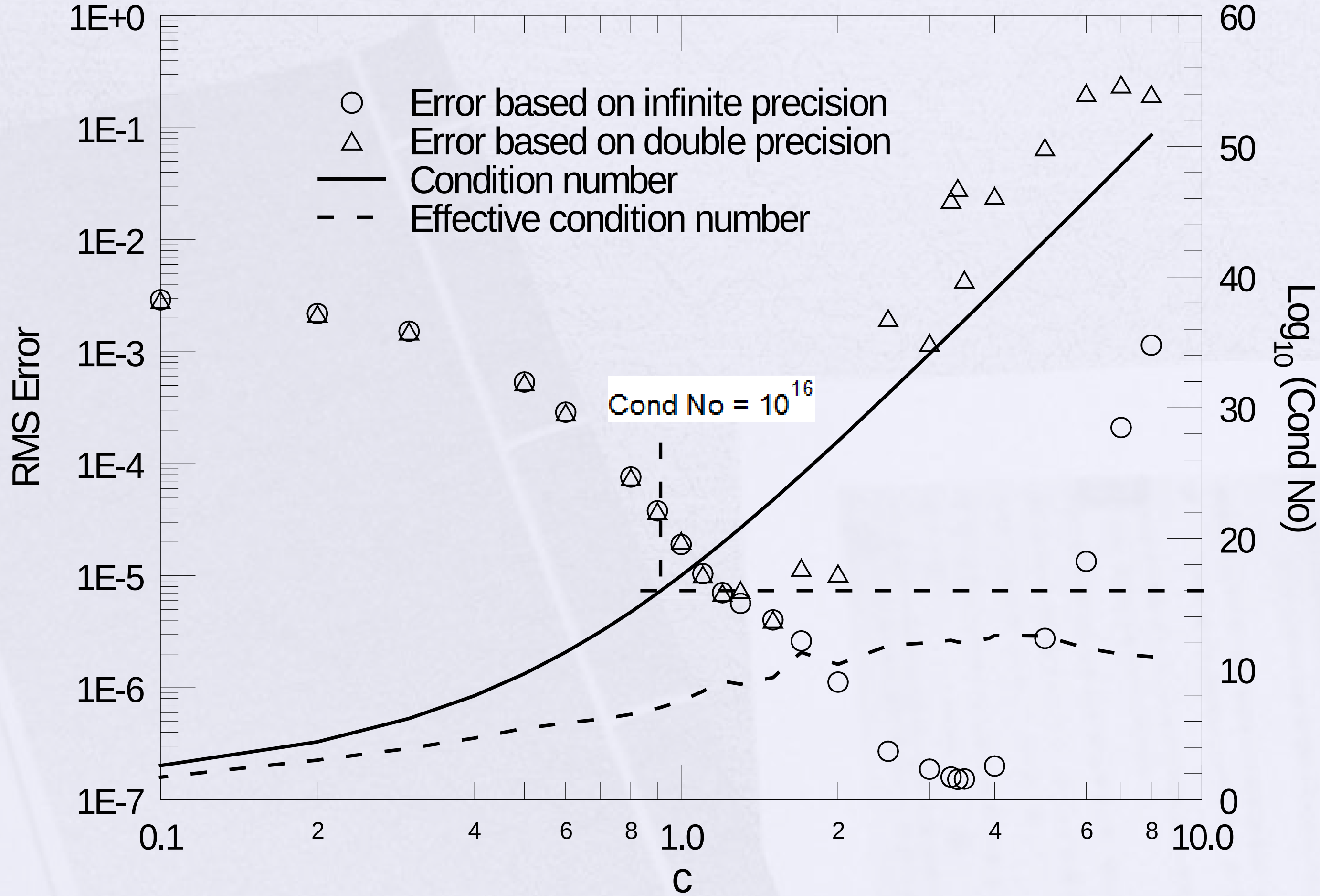


Figure 1: Root mean square errors (left axis) based on infinite and finite precision computation as compared to condition number and effective condition number, for inverse multiquadric interpolation of f_8, using $h = 0.1$ and various c values.

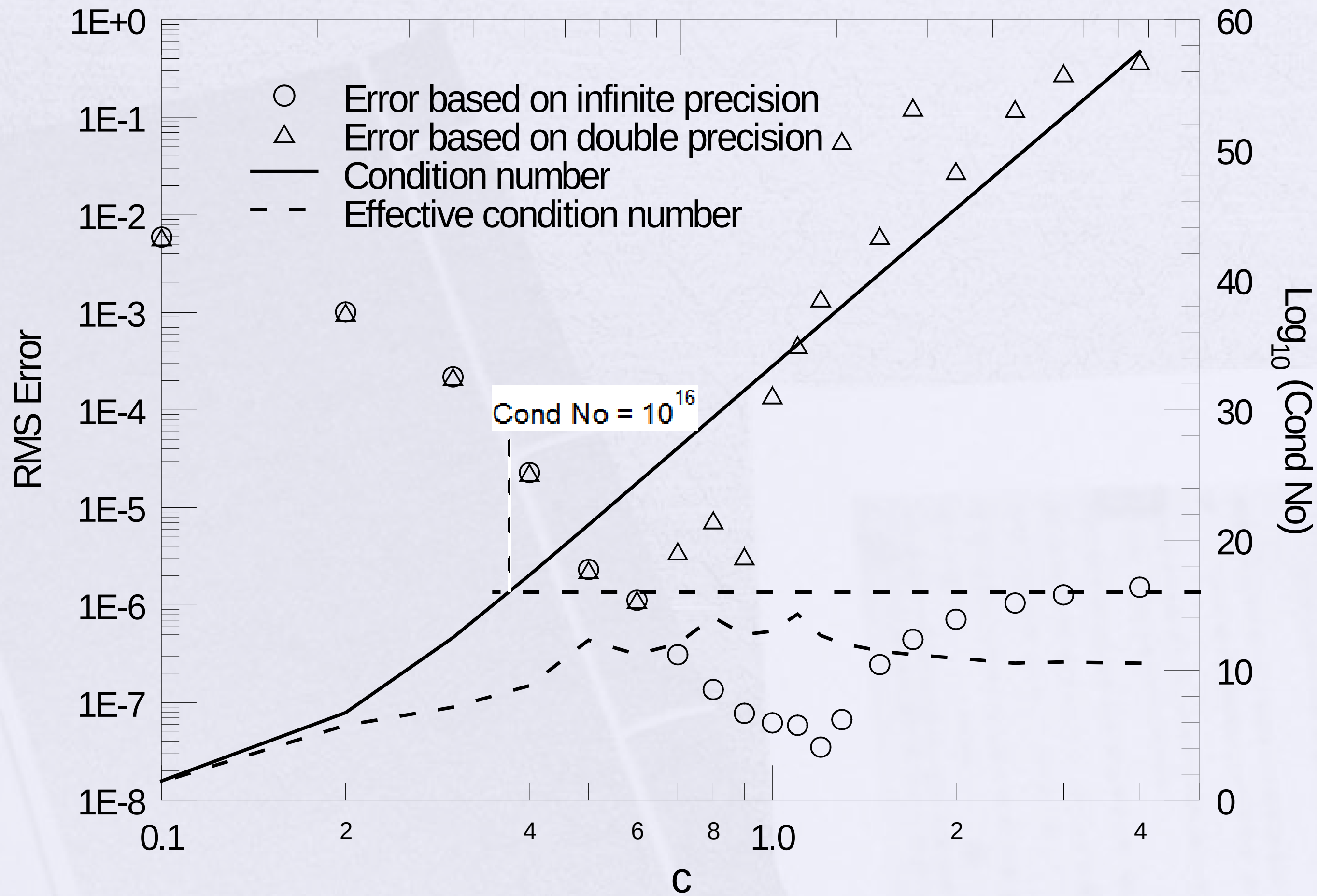


Figure 1: Root mean square errors (left axis) based on infinite and finite precision computation as compared to condition number and effective condition number, for Gaussian interpolation of f_8, using $h = 0.1$ and various c values.

IMQ						
c	Condition Number		$\|\alpha\|$		Interpolation RMS Error	
	κ	κ_{eff}	arbitrary precision	double precision	arbitrary precision	double precision
5.00	6.06E+42	3.39E+12	9.72E+28	1.23E+15	2.75E-06	6.73E-02
4.00	9.32E+38	3.74E+12	1.09E+25	4.29E+14	1.99E-07	2.48E-02
3.40	1.63E+36	1.16E+12	5.25E+22	1.94E+14	1.52E-07	2.92E-02
3.00	1.28E+34	1.02E+12	4.13E+20	8.09E+12	1.87E-07	1.20E-03
2.00	2.72E+27	2.27E+10	2.69E+15	3.82E+10	1.12E-06	1.05E-05
1.50	8.50E+22	2.17E+09	6.80E+11	5.29E+09	4.02E-06	4.07E-06
1.00	1.39E+17	3.42E+07	5.08E+07	2.27E+08	1.90E-05	2.05E-05
0.92	1.16E+16	1.22E+07	1.11E+07	1.46E+07	3.29E-05	3.31E-05
0.90	6.12E+15	9.68E+06	7.30E+06	7.00E+06	3.79E-05	3.78E-05
0.50	4.34E+09	2.79E+05	1.24E+02	1.24E+02	5.34E-04	5.34E-04
0.10	4.03E+02	5.11E+01	3.66E-02	3.66E-02	2.90E-03	2.90E-03

Table 13: Condition number and stability of interpolation coefficient α for IMQ interpolation.

Gauss						
c	Condition Number		$\|\alpha\|$		RMS error	
	κ	κ_{eff}	arbitrary precision	double precision	arbitrary precision	double precision
4.00	3.54E+57	3.34E+10	1.17E+45	1.37E+15	1.52E-06	3.78E-01
2.00	3.03E+45	8.53E+10	4.21E+32	9.60E+13	7.14E-07	2.83E-02
1.20	3.58E+36	4.52E+12	1.09E+22	5.86E+12	3.49E-08	1.40E-03
1.00	2.26E+33	1.00E+13	3.42E+18	3.90E+11	6.19E-08	1.42E-04
0.70	1.20E+27	1.06E+12	2.24E+13	6.04E+09	3.09E-07	3.57E-06
0.60	2.32E+24	1.68E+11	3.18E+11	1.43E+08	1.12E-06	1.13E-06
0.40	1.97E+17	6.18E+08	1.21E+07	1.45E+07	2.28E-05	2.28E-05
0.37	9.23E+15	1.72E+08	2.29E+06	2.29E+06	4.83E-05	4.83E-05
0.30	3.16E+12	1.39E+07	1.34E+04	1.34E+04	2.18E-04	2.18E-04
0.10	2.94E+01	2.49E+01	5.07E-01	5.07E-01	5.90E-03	5.90E-03

Table 14: Condition number and stability of interpolation coefficient α for GA interpolation

CONCLUSION

- Invertibility and (conditional) positive definiteness
- Error estimate with respect to fill distance
- Optimal shape parameter
- Polynomial limit as c -> infinity
- Error estimate with respect to shape parameter
- Theoretical upper bounds for condition number
- Effective condition number

- Round-off error and instability
- Derivative data and solution of PDE
- Runge (edge) effect