

Université Mohamed El Bachir El Ibrahimi de Bordj Bou Arréridj

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KAHOUL ZAKIYA

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**On the scattered data interpolation and approximation using radial
basis functions**

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DR- BERRAH ABDELMALEK Président

DR- ZEGHDANE REBIHA Encadreur

DR- DEKKAR KHADRA Examineur

DR-GUECHI AHMED Examineur

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To my father and my mother

To my family

To all my friends ...

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Introduction

The radial basis function (RBFs) is one of the primary tools for interpolating multidimensional scattered data. The methods ability to easily generalize to several spaces dimension, and provide spectral accuracy have made it particularly popular in several different type of applications [17]. Some of the more recent applications of these functions include cartography, neural networks, medical imaging, and the numerical solution of partial differential equations. The RBF interpolation matrix is very ill-conditioned to the average grid spacing h [1].

It was introduced in 1971 by Rolland Hardy [7]. He originally presented the method for the multiquadric (MQ)radial function. The method emerged from a cartography problem, where a bivariate interpolant of sparse and scattered data was needed to represent topography and produce contours. None of the existing interpolation methods (e.g. Fourier polynomial, bivariate splines) were satisfactory because they were either too smooth or too oscillatory. Furthermore, the non-singularity of their interpolation matrices was not guaranteed. In fact, Haar's theorem states the existence of a set of distinct nodes for which the interpolation matrix associated with node-independent basis functions is singular in two or higher dimensions [11]. In 1982, Richard Franke popularized the MQ method [6]. He subjected those methods to through tests, and found the MQ method overall to be the best one. Franke also conjectured the unconditional non-singularity of the interpolation matrix associated with the multiquadric radial function, but it was not until a few years later, in 1986, that Chareles Micchelli [10] was able to prove it. The main feature of the MQ method is that the interpolant is a linear combination of translations of basis function which only depends on the Euclidean distance from its center. This basis function is therefore radially symmetric with respect to its center. The MQ method was generalized to other "radial functions", such as the thin plate spline [3], the gaussian, the cubic, etc, and the method was called the "Radial Basis Function" method. In the 1990s the RBF was once again brought to the spotlight when Ed Kansa introduced a way to use it for solving parabolic, elliptic, and hyperbolic PDEs[8, 9]. Skala in 2016, described novel approaches based on RBFs for data interpolation and approximation generally in d-dimensional spaces [13].

The RBFs interpolation involves two stage. The first is fitting, solving a linear system corresponding to the interpolation conditions. The second is evaluation. In this work, we have taken

the direct approach of numerical experiments. First, we give some numerical tests of RBFs for solving some integral equations, the aim here is to give some remarks concerning the ill conditioned problem of the interpolation matrix and if this depends on the numerical accuracy of the approximations. Secondly, we examine if there is a relation between the shape parameter of the RBF and the condition number. The results obtained by the authors in [1], concerned the study of the matrix condition number $K(N, \alpha)$ and its asymptote function $k_{asymp}(\alpha)$ which is a function only of α and the RBF species, or to such a function multiplied by a power of N . For some RBFs it is possible to make highly plausible conjectures about the analytical form of $k_{asymp}(\alpha)$.

The dissertation is organized as follows, chapter one is divided into two parts, in the first, we introduce the problem of conditioning for a linear system or for a problem in general, and we give the interpolation problem in the second part.

In the second chapter, we will explain the problem of scattered data interpolation by the radial basis functions.

The last chapter is consacred to: Firstly, we present the problem of interpolation by the RBF function for solving nonlinear Volterra–Fredholm integral equations, and secondly through some numerical tests, we examine the condition number of some RBF functions. Finally, a conclusion is discussed in the last section of this dissertation.

Chapter 1

Conditioning of problem and interpolation

The subject of this chapter is to give some preliminary on the scattered data well conditioned problem and interpolation.

1.1 Phenomena of condition of problem

The phenomena of condition problem is one of the important problem in numerical analysis. We can view a problem as a function $f : X \rightarrow Y$ from a normed vector space X of data to a normed vector space Y of solution. This function f is usually nonlinear, but most of the time it is at least continuous. In generally, we shall be concerned with the behavior of a problem f at a particular data point $x \in X$ (the behavior may vary greatly from one point to another). A well-conditioned problem is one with the property that all small perturbations of x lead to only small changes in $f(x)$. An ill-conditioned problem is one with the property that some small perturbation of x leads to a large change in $f(x)$.

Remark 1.1 *So, we can describe the sensitivity of the solution to changes in the problem data as follows*

- *Well-conditioned problem:*
small changes in the data produce small changes in the solution.
- *Ill-conditioned (badly conditioned) problem:*
small changes in the data can produce large changes in the solution.

Example 1.1 *Let given the polynomial*

$$p(x) = (x - 1)(x - 2) \cdots (x - 10) + \delta.x^{10},$$

where δ is a parameter, we want to study the behavior of the roots of p for two values of δ . We

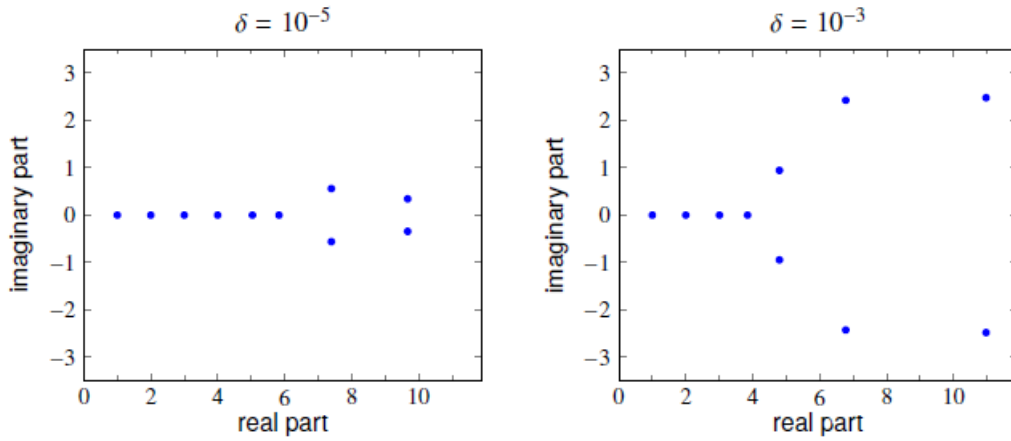


Figure 1.1: Roots of the polynomial p

can see from figure (1.1) that the problem is ill-conditioned.

1.1.1 Absolute and Relative condition

In this subsection, we give some properties of condition number of problem. Let δx denote a small perturbation of the variable x , we have

$$\delta f = f(x + \delta x) - f(x).$$

Definition 1.1

The absolute condition number $\kappa = \kappa(x)$ of f at x is defined as

$$\kappa = \lim_{\delta \rightarrow 0} \sup_{\|\delta x\| \leq \delta} \frac{\|\delta f\|}{\|\delta x\|}. \quad (1.1)$$

The limit of the supremum in the formula (1.1) can be interpreted as a supremum over all small perturbations δx . Generally, we can write

$$\kappa = \sup_{\delta x} \frac{\|\delta f\|}{\|\delta x\|}. \quad (1.2)$$

In the case where f is differentiable and from the definition of the derivative, we have $\delta f \approx J(x)\delta x$, with equality in the limit $\|\delta x\| \rightarrow 0$,

$$\kappa = \|J(x)\|. \quad (1.3)$$

where $\|J(x)\|$ represents the norm of the jacobian $J(x)$ induced by the norms on X and Y .

Definition 1.2 The relative condition number $\kappa_x = \kappa(x)$ is defined by

$$\kappa_x = \lim_{\delta \rightarrow 0} \sup_{\|\delta x\| \leq \delta} \left(\frac{\|\delta f\|}{\|f(x)\|} \bigg/ \frac{\|\delta x\|}{\|x\|} \right), \quad (1.4)$$

or, again assuming δx and δf are infinitesimal, we get

$$\kappa_x = \sup_{\delta x} \left(\frac{\|\delta f\|}{\|f(x)\|} \bigg/ \frac{\|\delta x\|}{\|x\|} \right). \quad (1.5)$$

If f is differentiable, we can express this quantity in terms of the jacobian as follows

$$\kappa_x = \frac{\|J(x)\|}{\|f(x)\|/\|x\|}. \quad (1.6)$$

Remark 1.2 The problem is well-conditioned if k is "small" (e.g., 1, 10, 10^2), and ill-conditioned if k is "large" (e.g., 10^6 , 10^{16}).

Example 1.2 Consider the problem of computing \sqrt{x} for $x > 0$. The jacobian of $f : x \mapsto \sqrt{x}$ is just the derivative $J = f' = \frac{1}{2\sqrt{x}}$, hence

$$\kappa = \frac{\|J(x)\|}{\|f(x)\|/\|x\|} = \frac{1/(2\sqrt{x})}{\sqrt{x}/x} = \frac{1}{2}.$$

This problem is well-conditioned.

Example 1.3

Consider the trivial problem of obtaining the scalar $\frac{x}{2}$ from $x \in \mathbb{C}$. We have

$$\kappa = \frac{\|J(x)\|}{\|f(x)\|/\|x\|} = \frac{1/2}{(x/2)/x} = 1.$$

This problem is well-conditioned.

Example 1.4

Consider the problem of obtaining the scalar $f(x) = x_1 - x_2$ from the vector $x = (x_1, x_2)^t \in \mathbb{C}^2$.

We use the infy -norm on the data space \mathbb{C}^2 . The jacobian of f is

$$J = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2} \right] = \left[1, -1 \right],$$

with $\|J\|_\infty = 2$, The condition number is given by

$$\kappa = \frac{\|J(x)\|_\infty}{\|f(x)\|/\|x\|} = \frac{2}{|x_1 - x_2|/\max(|x_1|, |x_2|)}.$$

This quantity is large if $|x_1 - x_2| \approx 0$, so the problem is ill-conditioned when $x_1 \approx x_2$.

1.1.2 Condition number of Matrix

Consider the problem of computing Ax from input x , we are going to determine the problem of condition number corresponding to perturbations of x but not A . We have

$$\kappa = \sup_{\delta x} \left(\frac{\|A(x + \delta x) - Ax\|}{\|Ax\|} \bigg/ \frac{\|\delta x\|}{\|x\|} \right) = \sup_{\delta x} \frac{\|A\delta x\|}{\|\delta x\|} \bigg/ \frac{\|Ax\|}{\|x\|}, \quad (1.7)$$

that is,

$$\kappa = \|A\| \frac{\|x\|}{\|Ax\|}. \quad (1.8)$$

Suppose in the above calculation that A is square and nonsingular. Then, we get

$$\kappa \leq \|A\| \|A^{-1}\|, \quad (1.9)$$

or $k = \alpha \|A\| \|A^{-1}\|$, with

$$\alpha = \frac{\|x\|}{\|Ax\|} \bigg/ \|A^{-1}\|.$$

For some choices of x , we get $\alpha = 1$ and

$$\kappa = \|A\| \|A^{-1}\|. \quad (1.10)$$

Theorem 1.1 [14] *Let $A \in \mathbb{C}^{m \times m}$ be nonsingular and consider the equation $Ax = b$. The problem of computing b , given x , has the condition number*

$$\kappa = \|A\| \frac{\|x\|}{\|b\|} \leq \|A\| \|A^{-1}\|, \quad (1.11)$$

with respect to perturbations of x . The problem of computing x , given b , has condition number

$$\kappa = \|A^{-1}\| \frac{\|b\|}{\|x\|} \leq \|A\| \|A^{-1}\|, \quad (1.12)$$

with respect to perturbation of b . If $\|\cdot\| = \|\cdot\|_2$, then equality holds in (1.11) if x is a multiple of a right singular vector of A corresponding to the minimal singular value σ_m , and equality holds in (1.12) if b is a multiple of a left singular vector of A corresponding to the maximal singular value σ_1 .

Definition 1.3 *The condition number of a matrix A , denoted by $\kappa(A)$ is defined as follows*

$$\kappa = \|A\| \|A^{-1}\|,$$

if $\kappa(A)$ is small, A is said to be well-conditioned, if $\kappa(A)$ is large, A is ill-conditioned. If A is singular, it is customary to write $\kappa(A) = \infty$.

Note that if $\|\cdot\| = \|\cdot\|_2$, then $\|A\| = \sigma_1$ and $\|A^{-1}\| = 1/\sigma_m$. Thus

$$\kappa(A) = \frac{\sigma_1}{\sigma_m}. \quad (1.13)$$

For a rectangular matrix $A \in \mathbb{C}^{m \times n}$ of full rank, $m \geq n$. The condition number is defined in terms of the pseudo-inverse (is a generalization of the matrix inverse when it is not invertible): $\kappa(A) = \|A\| \|A^+\|$.

1.1.3 Condition number of a system of equations

Let us hold b fixed and consider the behavior of the problem $A \mapsto x = A^{-1}b$, when A is perturbed by infinitesimal δA . Then x must change by infinitesimal δx . Let

$$(A + \delta A)(x + \delta x) = b.$$

Using the equality $Ax = b$ and dropping the doubly infinitesimal term $(\delta A)(\delta x)$. We obtain $(\delta A)x + A(\delta x) = 0$, that is $\delta x = -A^{-1}(\delta A)x$. This equation implies $\|\delta x\| \leq \|A^{-1}\| \|\delta A\| \|x\|$. or equivalently,

$$\frac{\|\delta x\|}{\|x\|} \bigg/ \frac{\|\delta A\|}{\|A\|} \leq \|A^{-1}\| \|A\| = \kappa(A). \quad (1.14)$$

Equality in this bound will hold whenever δA is such that

$$\|A^{-1}(\delta A)x\| = \|A^{-1}\| \|\delta A\| \|x\|, \quad (1.15)$$

and it can be shown by the use of dual norms that for any A and b and norm $\|\cdot\|$, such perturbation δA exist. This leads us to the following theorem.

Theorem 1.2 [14] *Let b be fixed and consider the problem of computing $x = A^{-1}b$, where A is square and nonsingular. The condition number of this problem with respect to perturbations in A is*

$$\kappa = \|A\| \|A^{-1}\| = \kappa(A).$$

Remark 1.3 *Theorem 1.1 and 1.2 are fundamental in numerical linear algebra, they determine how accurately one can solve systems of equations.*

Example 1.5

Let consider $Ax = b$ with

$$A = \begin{bmatrix} 1.01 & 0.99 \\ 0.99 & 1.01 \end{bmatrix}, \quad b = \begin{bmatrix} 2 \\ 2 \end{bmatrix},$$

where the exact solution is given by $x = [1, 1]^T$.

- Let's assume we computed a solution $\tilde{x} = [1.01, 1.01]^T$. Then the error

$$e = x - \tilde{x} = \begin{bmatrix} -0.01 \\ -0.01 \end{bmatrix},$$

is small, and the residual

$$r = b - Ax = \begin{bmatrix} 2 \\ 2 \end{bmatrix} - \begin{bmatrix} 2.02 \\ 2.02 \end{bmatrix} = \begin{bmatrix} -0.02 \\ -0.02 \end{bmatrix},$$

is also small.

- Now, let's assume that we computed a solution $\tilde{x} = [2, 0]^T$. This "solution" is obviously not a good one. Its error is

$$e = \begin{bmatrix} -1 \\ 1 \end{bmatrix},$$

which is quite large. However, the residual is

$$r = \begin{bmatrix} 2 \\ 2 \end{bmatrix} - \begin{bmatrix} 2.02 \\ 1.98 \end{bmatrix} = \begin{bmatrix} -0.02 \\ 0.02 \end{bmatrix},$$

which is still small. This is not good. This shows that the residual is not a reliable indicator of the accuracy of the solution.

1.1.4 Effect of Changes in A on the relative error

In this subsection, let consider the linear system $Ax = b$. But now A may be perturbed to $\tilde{A} = A + \delta A$. We suppose that x the exact solution of $Ax = b$, and \tilde{x} the exact solution of $\tilde{A}\tilde{x} = b$, i.e., $\tilde{x} = x + \delta x$.

This implies

$$\begin{aligned}\tilde{A}\tilde{x} = b &\iff (A + \delta A)(x + \delta x) = b \\ &\iff \underbrace{Ax - b}_{=0} + (\delta A)x + A(\delta x) + (\delta A)(\delta x) = 0.\end{aligned}$$

If we neglect the term with the product of the deltas then we get

$$(\delta A)x + A(\delta x) = 0 \quad \text{or} \quad (\delta x) = -A^{-1}(\delta A)x.$$

Taking norms this yields

$$\|\delta x\| \leq \|A^{-1}\| \|\delta A\| \|x\| \iff \|\delta x\| \leq \|A^{-1}\| \|A\| \frac{\|\delta A\|}{\|A\|} \|x\|,$$

or

$$\frac{\|x - \tilde{x}\|}{\|x\|} \leq \kappa(A) \frac{\|A - \tilde{A}\|}{\|A\|}.$$

The previous inequality can be interpreted as follows: For ill-conditioned matrices a small perturbation of the entries can lead to large changes in the solution of the linear system. This is a problem of an instability.

Example 1.6 *We consider*

$$A = \begin{bmatrix} 1.01 & 0.99 \\ 0.99 & 1.01 \end{bmatrix} \quad \text{with} \quad \delta A = \begin{bmatrix} -0.01 & 0.01 \\ 0.01 & -0.01 \end{bmatrix}.$$

Now

$$\tilde{A} = A + \delta A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix},$$

which is even singular, so that $\tilde{A}\tilde{x} = b$, with $b = [2, -2]^T$ has no solution at all.

1.1.5 Stability and Accuracy of a problem

The terms accuracy and precision are often confused or used interchangeably, but it is worth making a distinction between them. Accuracy refers to the absolute or relative error of an approximate quantity. Precision is the accuracy with which the basic arithmetic operations are performed. The distinction between forward and backward error, forward error is the most direct definition of error as the difference between the approximated and actual solution, but it is not always computable. Contrastingly, backward error is a calculable proxy for error

correlated with forward error.

Definition 1.4 (*Backward error*). *The backward error of an approximate solution to a numerical problem is the amount by which the problem statement would have to change to make the approximate solution exact.*

Example 1.7 *Suppose we write a function for finding square roots of positive numbers that outputs $\sqrt{2} \approx 1.4$. The forward error is $|1.4 - \sqrt{2}| \approx 0.0142$. The backward error is $|(1.4)^2 - 2| = 0.04$.*

Remark 1.4 • *The condition number of a problem can be seen as the ratio of how much its solution changes to the amount its statement changes under small perturbations. Alternatively, it is the ratio of forward to backward error for small changes in the problem statement.*

- *So, a problem is insensitive or well-conditioned when small amounts of backward error imply small amounts of forward error. In other words, a small perturbation to the statement of a well-conditioned problem yields only a small perturbation of the true solution.*

Definition 1.5 *An algorithm \tilde{f} for a problem f is stable if (for all x)*

$$\frac{\|\tilde{f}(x) - f(\tilde{x})\|}{\|f(\tilde{x})\|} = O(\epsilon_{\text{machine}}),$$

for some \tilde{x} with

$$\frac{\|\tilde{x} - x\|}{\|x\|} = O(\epsilon_{\text{machine}}).$$

Definition 1.6 *An algorithm \tilde{f} for a problem f is backward stable if (for all x)*

$$\tilde{f}(x) = f(\tilde{x}) \text{ for some } \tilde{x} \text{ with } \frac{\|\tilde{x} - x\|}{\|x\|} = O(\epsilon_{\text{machine}}).$$

Consider an algorithm \tilde{f} for a problem f . A computation $\tilde{f}(x)$ has absolute error $\|\tilde{f}(x) - f(x)\|$ and relative error

$$\frac{\|\tilde{f}(x) - f(x)\|}{\|f(x)\|}.$$

The algorithm is accurate if (for all x)

$$\frac{\|\tilde{f}(x) - f(x)\|}{\|f(x)\|} = O(\epsilon_{\text{machine}}).$$

1.2 Problem of interpolation

1.2.1 Polynomial interpolation

A fundamental mathematical technique is to approximate something complicated by something simple, or at least less complicated. This is the core idea of approximation with Taylor polynomials. The subject of using Taylor polynomial is that it approximates a given function well at a single point.

Definition 1.7 *The Taylor polynomial of f of degree n at a is noted by $T_n(f; a)$ and satisfies the conditions*

$$T_n(f; a)^{(i)}(a) = f^{(i)}(a), \text{ for } i = 0, 1, \dots, n. \quad (1.16)$$

The conditions in Taylor polynomial mean that $T_n(f, a)$ and f have the same value and first n derivatives at a . This makes it quite easy to derive an explicit formula for the Taylor polynomial.

Theorem 1.3 *The Taylor polynomial of f of degree n at a is unique and can be written as*

$$T_n(f; a)(x) = f(a) + (x - a)f'(a) + \frac{(x - a)^2}{2}f''(a) + \dots + \frac{(x - a)^n}{n!}f^{(n)}(a), \quad (1.17)$$

Derivation of the Taylor formula

We are going to prove theorem 1.3 in the quadratic case. Let

$$p_2(x) = c_0 + c_1x + c_2x^2. \quad (1.18)$$

that satisfies the conditions

$$p_2(a) = f(a), \quad p_2'(a) = f'(a), \quad p_2''(a) = f''(a). \quad (1.19)$$

The derivatives of p_2 are given by $p_2'(x) = c_1 + 2c_2x$ and $p_2''(x) = 2c_2$. Then we obtain

$$\begin{aligned} p_2(a) &= c_0 + c_1a + c_2a^2 = f(a) \\ p_2'(a) &= c_1 + 2c_2a = f'(a) \\ p_2''(a) &= 2c_2 = f''(a). \end{aligned} \quad (1.20)$$

This system is easy to solve. We have

$$\begin{aligned}c_2 &= f''(a)/2 \\c_1 &= f'(a) - 2c_2a = f'(a) - f''(a)a \\c_0 &= f(a) - c_1a - c_2a^2 = f(a) - (f'(a) - f''(a)a)a - f''(a)a^2/2,\end{aligned}$$

and then

$$\begin{aligned}p_2(x) &= f(a) - (f'(a) - f''(a)a)a - f''(a)a^2/2 + (f'(a) - f''(a)a)x + f''(a)x^2/2 \\&= f(a) + (x - a)f'(a) + (x^2 - 2ax + a^2)f''(a)/2 = f(a) + (x - a)f'(a) + (x - a)^2f''(a)/2.\end{aligned}$$

Remark 1.5 *In the derivation of the Taylor polynomial of degree n , the manipulations can be simplified if the polynomial is written as follows*

$$p_n(x) = c_0 + c_1(x - a) + c_2(x - a)^2 + \cdots + c_n(x - a)^n.$$

Theorem 1.4 [5] *Suppose that f is a function whose derivatives up to order $n + 1$ exist and are continuous. Then the remainder in the Taylor expansion*

$$R_n(f; a)(x) = f(x) - T_n(f; a)(x)$$

is given by

$$R_n(f; a)(x) = \frac{1}{n!} \int_a^x f^{(n+1)}(t)(x - t)^n dt. \quad (1.21)$$

The remainder may also be written as

$$R_n(f; a)(x) = \frac{(x - a)^{n+1}}{(n + 1)!} f^{(n+1)}(\xi), \quad (1.22)$$

where ξ is a number in the interval (a, x) (the interval (x, a) if $x < a$).

Example 1.8 *We want to determine a polynomial approximation of the function $\sin x$ on the interval $[-1, 1]$ at point $a = 0$, with error smaller than 10^{-5} . What we want to find is the smallest n such that*

$$\left| \frac{x^{n+1}}{(n + 1)!} f^{(n+1)}(\xi) \right| \leq 10^{-5},$$

where the function $f(x) = \sin x$ in our case and ξ is a number in the interval $(0, x)$. We want

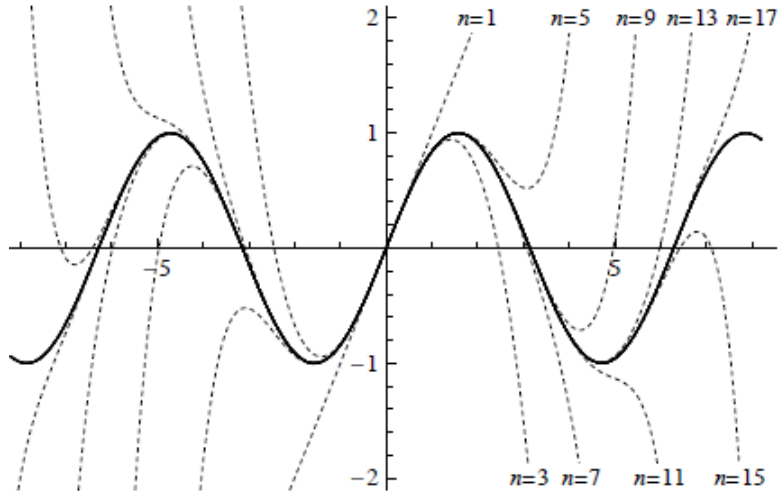


Figure 1.2: The Taylor polynomials of $\sin x$ (around $a = 0$) for degrees 1 to 17.

that the absolute value of the error should be smaller than 10^{-5} . We have

$$|f^{(n+1)}(\xi)| \leq 1.$$

and then

$$\left| \frac{x^{n+1}}{(n+1)!} f^{(n+1)}(\xi) \right| \leq \frac{|x|^{n+1}}{(n+1)!} \leq 10^{-5},$$

Since $x \in [-1, 1]$ we know that $|x| \leq 1$ so this last inequality will be satisfied if

$$\frac{1}{(n+1)!} \leq 10^{-5}.$$

We find an n that satisfies this last inequality we see that.

When

$$n = 8, \text{ we have } 1/8! \approx 2.5 \times 10^{-5}.$$

$$n = 9, \text{ we have } 1/9! \approx 2.8 \times 10^{-6}.$$

This means that the smallest value of n is $n = 8$. Then the Taylor polynomial is given by

$$p_8(x) = T_8(\sin x; 0) = x - \frac{x^3}{3} + \frac{x^5}{120} - \frac{x^7}{5040},$$

since the term of degree 8 is zero. If we evaluate this we find $p_8(1) \approx 0.841468$ with error roughly 2.73×10^{-6} which is close to the estimate $1/9!$ which we computed above.

Figure (1.2) shows the Taylor polynomials of $\sin x$ about $a = 0$ of degree up to 17. In particular we see that for degree 7, the approximation is indistinguishable from the original in the plot, at least up to $x = 2$.

Corollary 1.1

Any function f whose first $n + 1$ derivatives are continuous at $x = a$ can be expanded in a Taylor polynomial of degree n at $x = a$ with a corresponding error term,

$$f(x) = f(a) + (x - a)f'(a) + \cdots + \frac{(x - a)^n}{n!}f^n(a) + \frac{(x - a)^{n+1}}{(n + 1)!}f^{n+1}(\xi_x), \quad (1.23)$$

where ξ_x is a number in the interval (a, x) (the interval (x, a) if $x < a$) that depends on x . This is called a Taylor expansion of f .

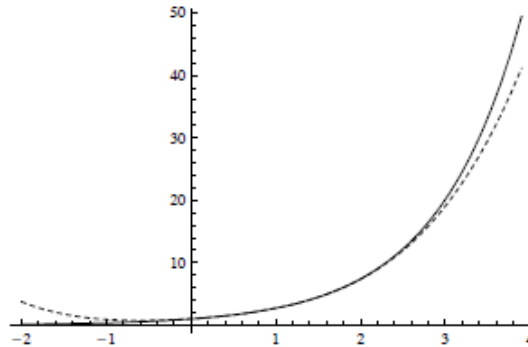


Figure 1.3: Taylor polynomial of degree 4 about the point $a = 1$ for the function $f(x) = \exp(x)$.

Example 1.9 Figure (1.3) shows a plot of the Taylor polynomial of degree 4 for the exponential function $f(x) = \exp(x)$, expanded about the point $a = 1$. For this function it is easy to see that the Taylor polynomials will converge to $\exp(x)$ on any interval as the degree tends to infinity.

1.2.2 Interpolation by Newton polynomial

A Taylor polynomial based at a point $x = a$ usually provides a very good approximation near a , but as we move away from this point, the error will increase. The aim here is to obtain a good approximation to a function f across a whole interval. This is done by interpolation. We approximate a function f by a polynomial p by forcing p to have the same function values as f at a number of points. Suppose that we have $n + 1$ distinct points $(x_i)_{i=0}^n$ scattered throughout the interval $[a, b]$ where scattered f is defined. Since a polynomial of degree n has $n + 1$ free coefficients it is natural to try and find a polynomial of degree n with the same values as f at these points.

Let f be a given function defined on an interval $[a, b]$, and let $(x_i)_{i=0}^n$ be $n + 1$ distinct points in $[a, b]$. The polynomial interpolation problem is to find a polynomial $p_n = P(f; x_0, \dots, x_n)$ of degree n that matches f at the given points,

$$p_n(x_i) = f(x_i), \text{ for } i = 0, 1, \dots, n. \quad (1.24)$$

The points $(x_i)_{i=0}^n$ are called interpolation points, and the polynomial $p_n = P(f; x_0, \dots, x_n)$ is called a polynomial interpolant. One of the most known of polynomial interpolation is Newton interpolation polynomial.

Newton form of the interpolating polynomial

Definition 1.8 Let $(x_i)_{i=0}^n$ be $n + 1$ distinct real numbers. The Newton form of a polynomial of degree n is given by

$$p_n(x) = c_0 + c_1(x - x_0) + c_2(x - x_0)(x - x_1) + \dots + c_n(x - x_0)(x - x_1) \cdots (x - x_{n-1}). \quad (1.25)$$

Example 1.10 (Newton form for $n = 0$) Suppose we have only one interpolation point x_0 . Then the Newton form is just $p_0(x) = c_0$. To interpolate f at x_0 , we have $c_0 = f(x_0)$, and then $p_0(x) = f(x_0)$.

Example 1.11 (Newton form for $n = 1$) With two points x_0 and x_1 the Newton form is $p_1(x) = c_0 + c_1(x - x_0)$. Interpolation at x_0 means that

$$f(x_0) = p_1(x_0) = c_0$$

and interpolate at x_1 , we get

$$f(x_1) = p_1(x_1) = f(x_0) + c_1(x_1 - x_0),$$

which means that

$$c_0 = f(x_0), \quad c_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}. \quad (1.26)$$

We note that c_0 remains the same as in the case $n = 0$.

In general, we have

$$f(x_0) = c_0,$$

$$f(x_1) = c_0 + c_1(x_1 - x_0),$$

$$f(x_2) = c_0 + c_1(x_2 - x_0) + c_2(x_2 - x_0)(x_2 - x_1),$$

$$f(x_3) = c_0 + c_1(x_3 - x_0) + c_2(x_3 - x_0)(x_3 - x_1) + c_3(x_3 - x_0)(x_3 - x_1)(x_3 - x_2),$$

⋮

$$f(x_k) = c_0 + c_1(x_k - x_0) + \dots + c_{k-1}(x_k - x_0) \cdots (x_k - x_{k-2}) + c_k(x_k - x_0) \cdots (x_k - x_{k-1}).$$

This is an example of a triangular system, each coefficient c_k only depends on the data $(x_0, f(x_0)), (x_1, f(x_1)), \dots, (x_k, f(x_k))$, and we have the following theorem.

Theorem 1.5 *Let f be a given function and x_0, \dots, x_n are distinct interpolation points. There is a unique polynomial of degree n which interpolates f at these points. If the interpolating polynomial is expressed in Newton form,*

$$p_n(x) = c_0 + c_1(x - x_0) + \dots + c_n(x - x_0)(x - x_1) \cdots (x - x_{n-1}), \quad (1.27)$$

then c_k depends only on $(x_0, f(x_0)), (x_1, f(x_1)), \dots, (x_k, f(x_k))$ which is indicated by the notation

$$c_k = f[x_0, \dots, x_k], \quad (1.28)$$

for $k = 0, 1, \dots, n$. The interpolating polynomials p_n and p_{n-1} are related by

$$p_n(x) = p_{n-1}(x) + f[x_0, \dots, x_n](x - x_0) \cdots (x - x_{n-1}).$$

Using (1.28) for the coefficients, the interpolation formula (1.27) becomes

$$p_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + \dots + f[x_0, \dots, x_n](x - x_0) \cdots (x - x_{n-1}). \quad (1.29)$$

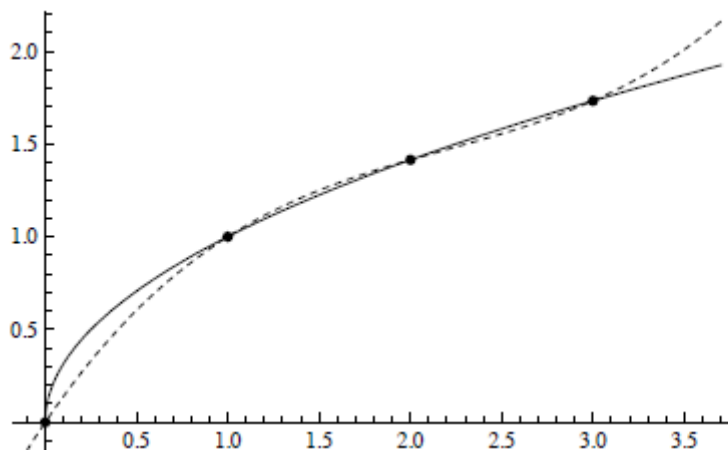


Figure 1.4: The function $f(x) = \sqrt{x}$ (solid) and its cubic interpolant at the four points 0, 1, 2, and 3 (dashed).

Example 1.12 *Suppose we have the four points $x_i = i$, for $i = 0, \dots, 3$, and we want to interpolate the function \sqrt{x} at these points. In this case the Newton form is given by*

$$p_3(x) = c_0 + c_1x + c_2x(x - 1) + c_3x(x - 1)(x - 2).$$

The interpolation conditions are as follows

$$\begin{aligned}
 0 &= c_0, \\
 1 &= c_0 + c_1, \\
 \sqrt{2} &= c_0 + 2c_1 + 2c_2, \\
 \sqrt{3} &= c_0 + 3c_1 + 6c_2 + 6c_3.
 \end{aligned} \tag{1.30}$$

We solve the system (1.30), we obtain

$$c_0 = 0, c_1 = 1, c_2 = -(1 - \sqrt{2}/2), c_3 = (3 + \sqrt{3} - 3\sqrt{2})/6.$$

Figure (1.4) shows a plot of this interpolant.

Theorem 1.6 [2] Let $c_k = f[x_0, \dots, x_k]$, denote the leading coefficient of the interpolating polynomial $P(f, x_0, \dots, x_k)$. This is called a k^{th} order divided difference of f and satisfies the relations $f[x_0] = f(x_0)$, and

$$f[x_0, \dots, x_k] = \frac{f[x_1, \dots, x_k] - f[x_0, \dots, x_{k-1}]}{x_k - x_0}, \tag{1.31}$$

for $k > 0$.

The divided differences can be given as follows

$$\begin{array}{ccccccc}
 x_0 & f[x_0] & & & & & \\
 x_1 & f[x_1] & f[x_0, x_1] & & & & \\
 x_2 & f[x_2] & f[x_1, x_2] & f[x_0, x_1, x_2] & & & \\
 x_3 & f[x_3] & f[x_2, x_3] & f[x_1, x_2, x_3] & f[x_0, x_1, x_2, x_3] & & \\
 \vdots & & & & & &
 \end{array} . \tag{1.32}$$

Example 1.13 Suppose, we have the data

x	0	1	2	3
$f(x)$	0	1	1	2

Then

x	$f(x)$			
0	0			
1	1	1		
2	1	0	-1/2	
3	2	1	1/2	1/3

This means that the interpolating polynomial is

$$\begin{aligned}
 p_3(x) &= 0 + 1(x - 0) - \frac{1}{2}(x - 0)(x - 1) + \frac{1}{3}(x - 0)(x - 1)(x - 2) \\
 &= x - \frac{1}{2}x(x - 1) + \frac{1}{3}x(x - 1)(x - 2).
 \end{aligned}$$

A plot of this polynomial with the interpolation points is shown in figure (1.5).

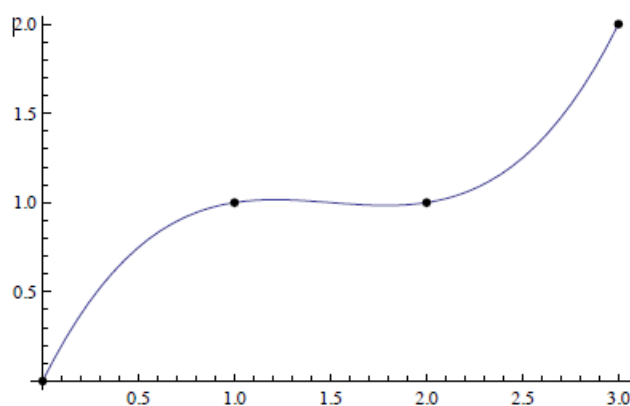


Figure 1.5: The data points and the interpolant.

Theorem 1.7 [2] Let f be a function whose first k derivatives are continuous in the smallest interval $[a, b]$ that contains all the numbers x_0, \dots, x_k . Then

$$f[x_0, \dots, x_k] = \frac{f^{(k)}(\xi)}{k!}, \quad (1.33)$$

where $\xi \in (a, b)$.

1.2.3 Interpolation error and Runge phenomena

Theorem 1.8 Suppose f is interpolated by a polynomial of degree n at $n + 1$ distinct points x_0, \dots, x_n . Let $[a, b]$ be the smallest interval that contains all the interpolation points as well as the number x , and suppose that the function f has continuous derivatives up to order $n + 1$

in $[a, b]$. Then the error $e(x) = f(x) - p_n(x)$ is given by

$$e(x) = f[x_0, \dots, x_n, x](x - x_0) \cdots (x - x_n) = \frac{f^{(n+1)}(\xi_x)}{(n+1)!} (x - x_0) \cdots (x - x_n), \quad (1.34)$$

where ξ_x is a number in the interval (a, b) that depends on x .

Proof 1 First, we need to prove the first equality. For this we add the (arbitrary) number x as an interpolation point and consider interpolation with a polynomial of degree $n + 1$ at the points x_0, \dots, x_n, x . We have

$$p_{n+1}(t) = p_n(t) + f[x_0, \dots, x_n, x](t - x_0) \cdots (t - x_n).$$

Since p_{n+1} interpolates f at $t = x$ we have $p_{n+1}(x) = f(x)$ so

$$f(x) = p_n(x) + f[x_0, \dots, x_n, x](x - x_0) \cdots (x - x_n),$$

which proves the first relation in (1.34) and the prove of the second inequality is given by theorem 1.7.

Runge's phenomenon

Runge's phenomenon is a problem of oscillation at the edges of an interval that occurs when using polynomial interpolation with polynomials of high degree over a set of equispaced interpolation points. It was discovered by Carl David Tolmé Runge when exploring the behavior of errors when using polynomial interpolation to approximate certain functions. The discovery was important because it shows that going to higher degrees does not always improve accuracy. The Weierstrass approximation theorem confirm that every continuous function $f(x)$ defined on an interval $[a, b]$ can be uniformly approximated by a polynomial function $P_n(x)$ of sufficiently large degree $\leq n$, i.e.,

$$\lim_{n \rightarrow \infty} (\max_{a \leq x \leq b} |f(x) - P_n(x)|) = 0.$$

Runge's phenomenon demonstrates, however, that interpolation can easily result in divergent approximations.

The Runge phenomena is as follows, let consider the function:

$$f(x) = \frac{1}{1 + 25x^2}.$$

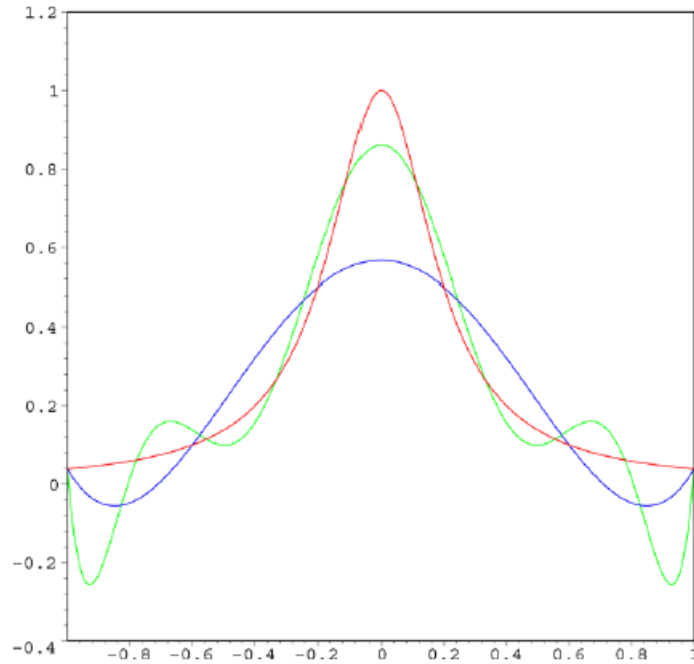


Figure 1.6: The red curve is **the Runge function**. The blue curve is **a 5th-order interpolating polynomial**. The green curve is **a 9th-order interpolating polynomial**.

Runge show that if this function is interpolated at equidistant points x_i between -1 and 1 such that:

$$x_i = \frac{2i}{n} - 1, \quad i \in \{0, 1, \dots, n\}.$$

with a polynomial $P_n(x)$ of degree $\leq n$, the resulting interpolation oscillates toward the end of the interval which is presented in figure (1.6). It can be proven that the interpolation error increases when the degree of the polynomial is increased which signify that

$$\lim_{n \rightarrow \infty} \left(\max_{-1 \leq x \leq 1} |f(x) - P_n(x)| \right) = +\infty.$$

The error between the generating function and the interpolating polynomial of order n is given by

$$\max_{-1 \leq x \leq 1} |f(x) - P_n(x)| \leq \max_{-1 \leq x \leq 1} \frac{|f^{n+1}(x)|}{n+1!} \max_{-1 \leq x \leq 1} \prod_{i=0}^n |x - x_i|$$

For the case of the Runge function, interpolated at equidistant points, each of the two multipliers in the upper bound for the approximation error grows to infinity with n .

Mitigations to the problem

- The oscillation can be minimized by using nodes that are distributed more densely towards the edges of the interval, specifically, with asymptotic density (on the interval $[-1,1]$) given by $1/\sqrt{1-x^2}$. A standard example of such a set of nodes is Chebyshev nodes, for which the maximum error in approximating the Runge function is guaranteed to diminish with

increasing polynomial order. The phenomenon demonstrates that high degree polynomials are generally unsuitable for interpolation with equidistant nodes.

- The problem can be avoided by using spline curves which are "piecewise polynomials". When trying to decrease the interpolation error one can increase the number of polynomial pieces which are used to construct the spline instead of increasing the degree of the polynomials used.
- We can also use "fitting a polynomial" technique of lower degree using the method of least squares. Generally, when using m equidistant points, if $N < 2\sqrt{m}$ then least squares approximation $P_N(x)$ is well-conditioned.

Chapter 2

Interpolation with radial basis functions

2.1 The Scattered Data Interpolation

In practical applications we have to face the problem of reconstructing an unknown function f from a set (usually small) of data. These data consist of two sets: the data sites $X = x_1, \dots, x_N$ and the data values $f_j = f(x_j), j = 1, \dots, N$. The reconstruction has to approximate the data values at the data sites. In practice we are looking for a function s that either interpolates the data, i.e. it satisfies the conditions $s(x_j) = f_j; 1 \leq j \leq N$ or approximate the data, i.e. $s(x_j) \approx f_j$.

In many cases the data are scattered, that is they have no special structure. Moreover in several applications the data sites are considered in high dimension. Hence, for a unifying approach, methods have been developed in the last decades with the aim to meet all these (new) situations. We suppose that the data sites are ordered as follows:

$$X : a < x_1 < x_2 < \dots < x_N < b, \tag{2.1}$$

with corresponding data values f_1, \dots, f_N to be interpolated at the data set X . The problem is to find $s : [a; b] \rightarrow \mathbb{R}$ with the property $s(x_j) = f_j$ for all $j = 1, \dots, N$. In the univariate setting, a simple solution of the above problem consists in taking s as polynomial p of degree at most $N - 1$, but solution is not working in higher dimensions. The main reasons why we are interested on such a problem in our setting are:

- Scattered data fitting is a fundamental problem in approximation theory and data modeling in general.
- Mathematical challenge: we want a well-posed problem formulation.

- This will naturally lead to distance matrices
- Later we generalize to radial basis functions or positive definite kernels

In the univariate setting it is well known that one can interpolate to arbitrary data at N distinct data sites using a polynomial of degree $N - 1$. For the multivariate setting, however, there is the following negative result (see [Mairhuber (1956); Curtis (1959)]).

Definition 2.1 Haar space *Suppose that $\Omega \subseteq \mathbb{R}^d$ contains at least N points. Let $V \subseteq C(\Omega)$ can be an N -dimensional linear space. Then V is called a Haar space of dimension N on Ω if for arbitrary distinct points x_1, \dots, x_N and arbitrary f_1, \dots, f_N there exists exactly one function $s \in V$ with $s(x_i) = f_i, \quad 1 \leq i \leq N$.*

Theorem 2.1 *Under the conditions of definition 2.1 the following statements are equivalent.*

1. V is an N -dimensional Haar space.
2. Every $u \in V \setminus \{0\}$ has at most $N - 1$ zeros.
3. For any distinct points $x_1, \dots, x_N \in \Omega$ and any basis u_1, \dots, u_N of V we have that

$$\det(u_j(x_i)) \neq 0.$$

Proof 2 *Suppose that V is an N -dimensional Haar space and $u \in V \setminus \{0\}$ has N zeros, say x_1, \dots, x_N . In this case u and the zero function both interpolate zero on these N points. From the uniqueness we can conclude that $u \equiv 0$ in contrast with our assumption.*

Next, let us assume that the second property is satisfied. If $\det A = 0$ with $A = (u_j(x_i))$ then there exists a vector $\alpha \in \mathbb{R}^N \setminus \{0\}$ with $A\alpha = 0$, i.e.

$$\sum_{j=1}^N \alpha_j u_j(x_i) = 0, \quad \text{for } 1 \leq i \leq N.$$

This means that the function $u = \sum \alpha_j u_j$, has N zeros and must therefore be identically zero. This is impossible since $\alpha \neq 0$.

Finally, if the third property is satisfied then we can make $u = \sum \alpha_j u_j$, for the interpolant. Obviously, the interpolation conditions become

$$\sum_{j=1}^N \alpha_j u_j(x_i) = f_i, \quad 1 \leq i \leq N.$$

Now the coefficient vector, and hence u , is uniquely determined because $A = (u_j(x_i))$ is nonsingular.

Theorem 2.2 Mairhuber-Curtis

Suppose that $\Omega \subseteq \mathbb{R}^d, d \geq 2$, contains an interior point. Then there exists no Haar space on Ω of dimension $N \geq 2$.

Proof 3 Suppose that $U = \text{span}\{u_1, \dots, u_N\}$ is a Haar space on Ω . As Ω contains an interior point there exists a ball $B(x_0, \delta) \subseteq \Omega$ with radius $\delta > 0$ and we can fix pairwise distinct $x_3, \dots, x_N \in B(x_0, \delta)$. Next we choose two continuous curves $x_1(t), x_2(t), t \in [0, 1]$ such that $x_1(0) = x_2(1), x_1(1) = x_2(0)$ and such that the curves neither have any other points of intersection nor have any common points with $\{x_3, \dots, x_N\}$. This is possible since $d \geq 2$. Then on the one hand, since U is assumed to be a Haar space on Ω , the function

$$D(t) := \det((u_j(x_k))_{1 \leq j, k \leq N}),$$

is continuous and does not change sign. On the other hand $D(1) = -D(0)$ because only the first two rows of the involved matrices are exchanged. Thus D must change signs, which is a contradiction.

Note that existence of a Haar space guarantees invertibility of the interpolation matrix A , i.e., existence and uniqueness of an interpolant. As mentioned above, univariate polynomials of degree $N - 1$ form an N -dimensional Haar space for data given at x_1, \dots, x_N .

Mairhuber-Curtis theorem tells us that if we want to have a well-posed multivariate scattered data interpolation problem we can no longer fix in advance the set of basis functions for arbitrary scattered data. For example, it is not possible to perform unique interpolation with (multivariate) polynomials of degree N to data given at arbitrary locations in \mathbb{R}^2 . Instead, the basis should depend on the data locations.

Indeed it is a well-established fact that a large data set is better dealt with splines than by polynomials. The accuracy of the interpolation process using splines is not on the polynomial degree but on the spacing of the data sites. The set of cubic splines corresponding to the subdivision (2.1) is the space

$$S_3(X) = \{s \in C^2[a, b] : s_{[x_i, x_{i+1}]} \in P_3 \in (\mathbb{R}), 0 \leq i \leq N\}, \quad (2.2)$$

with $a = x_0$ and $x_{N+1} = b$. The space $S_3(x)$ has dimension $N + 4$ and hence the interpolation condition $(s(x_i) = f_i, 1 \leq i \leq N)$ not sufficient to guarantee a unique interpolant. To enforce uniqueness, in the case of natural splines, i.e. the set

$$N_3(X) = \{s \in S_3(x) : s_{|[a, x_1]}, s_{|[x_N, b]} \in P_1(\mathbb{R})\}, \quad (2.3)$$

that consists of all cubic splines that are linear polynomials on the outer intervals $[a, x]$ and $[x_N, b]$. It come easy to see that a cubic spline s is a natural spline if and only if it satisfies $s''(x_1) = s^{(3)}(x_1) = 0$ and $s''(x_N) = s^{(3)}(x_N) = 0$. With this choice we have imposed 4 additional conditions to the space, so it is natural to assume that the $\dim(N_3(X)) = N$. So, the initial interpolation problem has a unique solution in $N_3(X)$. This approach has allowed to develop a beautiful theory where all space dimensions can be handled in the same way. The resulting approximation spaces no longer consist of piecewise polynomials, so they can not be called splines. The new functions are known Radial Basis Functions (RBF).

2.1.1 Cubic splines to RBF

To get a good idea, let the set $S_3(X)$ has the basis of truncated powers $(x - x_j)_+^3, 1 \leq j \leq N$ plus an arbitrary basis for $P_3(\mathbb{R})$. Hence every $s \in N_3(X)$ can be represented in the form

$$s(x) = \sum_{j=1}^N a_j (x - x_j)_+^3 + \sum_{j=0}^3 b_j x^j, x \in [a, b]. \quad (2.4)$$

Because s is a natural spline we have the additional information that s is linear on the two outer intervals. That is on $[a, x_1]$ the spline is simply $s(x) = b_0 + b_1 x$ (since $b_2 = b_3 = 0$).

Thus (2.4) becomes

$$s(x) = \sum_{j=1}^N a_j (x - x_j)_+^3 + b_0 + b_1 x, x \in [a, x_1] \quad (2.5)$$

To derive the representation of s in $[x_N; b]$ we have simply to remove all subscripts $+$ on the functions $(x - x_j)_+^3$ in (2.5). Expanding these cubics and rearranging the sums we get

$$s(x) = \sum_{k=0}^3 \binom{3}{k} (-1)^{3-k} \left(\sum_{j=1}^N a_j x_j^{3-k} \right) x^k + b_0 + b_1 x, x \in [x_N, b]. \quad (2.6)$$

Thus, for s to be a natural spline, the coefficients of s have to satisfy

$$\sum_{j=1}^N a_j = \sum_{j=1}^N a_j x_j = 0. \quad (2.7)$$

This is a first characterization of natural cubic splines.

One more step. Using the identity $x_+^3 = \frac{(|x|^3+x^3)}{2}$, and the relation (2.4), get

$$\begin{aligned} s(x) &= \sum_{j=1}^N \frac{a_j}{2} |x - x_j|^3 + \sum_{j=1}^N \frac{a_j}{2} (x - x_j)^3 + b_0 + b_1 x \\ &= \sum_{j=1}^N \frac{a_j}{2} |x - x_j|^3 + \sum_{k=0}^3 \binom{3}{k} (-1)^{3-k} \left(\sum_{j=1}^N a_j x_j^{3-k} \right) x^k + b_0 + b_1 x \\ &= \sum_{j=1}^N \hat{a}_j |x - x_j|^3 + \hat{b}_0 + \hat{b}_1 x, \end{aligned}$$

where $\hat{a}_j = a_j/2, 1 \leq j \leq N, \hat{b}_0 = b_0 - \frac{1}{2} \sum_{j=1}^N a_j x_j^3$ and $\hat{b}_1 = b_1 + \frac{3}{2} \sum_{j=1}^N a_j x_j^2$.

Proposition 2.1 *Every natural spline s has the representation*

$$s(x) = \sum_{j=1}^N a_j \phi(|x - x_j|) + p(x), x \in \mathbb{R}, \quad (2.8)$$

where $\phi(r) = r^3, r \geq 0$ and $p \in \mathbb{P}_1(\mathbb{R})$. On the contrary, for every set $X = \{x_1, \dots, x_N\}$ of pairwise distinct points and for every $f \in \mathbb{R}$ there exists a function s of the form (2.4), which interpolates the data, i.e. $s(x_j) = f(x_j), 1 \leq j \leq N$.

The generalization to \mathbb{R}^d is straightforward where the name "radial" becomes even more evident.

In fact

$$s(x) = \sum_{j=1}^N a_j \phi(\|x - x_j\|_2) + p(x), x \in \mathbb{R}^d, \quad (2.9)$$

where $\phi : [0; \infty) \rightarrow \mathbb{R}$ is a univariate fixed function and $p \in \mathbb{P}_{m-1}(\mathbb{R}^d)$ is a low degree polynomial. The additional conditions on the coefficients become

$$\sum_{j=1}^N a_j q(x_j) = 0, \forall q \in \mathbb{P}_{m-1}(\mathbb{R}^d). \quad (2.10)$$

In many cases, we can avoid the condition (2.10), in these cases the interpolation problem has solution if

$$A_{\phi, X} := (\phi\|x_i - x_j\|_2)_{1 \leq i, j \leq N},$$

is invertible. We can ask the question: Does there exist a function $\phi : [0; \infty) \rightarrow \mathbb{R}$ such that for all $d; N \in \mathbb{N}$ and all pairwise distinct $x_1, \dots, x_n \in \mathbb{R}^d$, the matrix $A_{\phi, X}$ is nonsingular?. The answer is affirmative. Examples of functions that allow to build matrices nonsingular are: the gaussians $\phi(r) = e^{-\alpha r^2}, \alpha > 0$, the inverse multiquadric $\phi(r) = (c^2 + r^2)^{-1/2}$ and the

multiquadric $\phi(r) = (c^2 + r^2)^{1/2}; c > 0$. In the two first cases it is even true that the matrix $A_{\phi,X}$ is always positive definite (and so invertible).

Definition 2.2 A function $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ is called radial provided there exists a univariate function $\Phi : [0, \infty) \rightarrow \mathbb{R}$ such that

$$\phi(x) = \Phi(r),$$

where $r = \|x\|$, and $\|\cdot\|$ is some norm on \mathbb{R}^d usually the Euclidean norm. Some radial basis functions are given in table (2.1) and figures (2.1)-(2.2).

$\phi(r)$	Name	Abbreviation	Polynomial part
$\sqrt{1 + \varepsilon^2 r^2}$	Multiquadrics	MQ	None
$(1 + \varepsilon^2 r^2)^{m/2}$	Generalized MQ	GMQ	Degree $(m - 2)$
$1/\sqrt{\varepsilon^2 r^2 + 1}$	Inverse multiquadrics	IMQ	None
$(\varepsilon^2 r^2 + 1)^{-m/2}$	Generalized IMQ	GIMQ	None
$1/(1 + \varepsilon^2 r^2)$	Inverse quadratic	IQ	None
$\exp(-\varepsilon^2 r^2)$	Gaussians	GA	None
$\text{sech}(\varepsilon r)$	Sech	SH	None
$r^2 \log(r)$	Thin plate splines	TPS2	Linear
$r^4 \log(r)$	Thin plate splines	TPS4	Quadratic
$r^{2m} \log(r)$	Thin plate splines	TPS	Degree m
r^3	Cubic	MN3	Linear
r^5	Quintic	MN5	Quadratic
r^{2m+1}	Monomial	MN	Degree m

Table 2.1: Radial basis functions: definitions and polynomial augmentation.

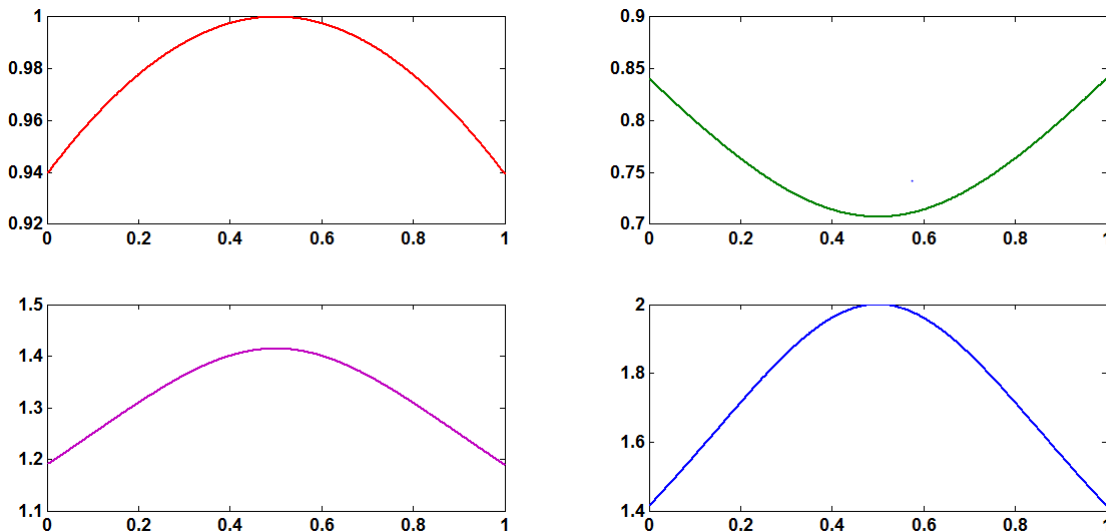


Figure 2.1: Gaussian RBF (left), Multiquadric (right), Inverse multiquadric (left), Quadric (right) for the center $x=1/2$.

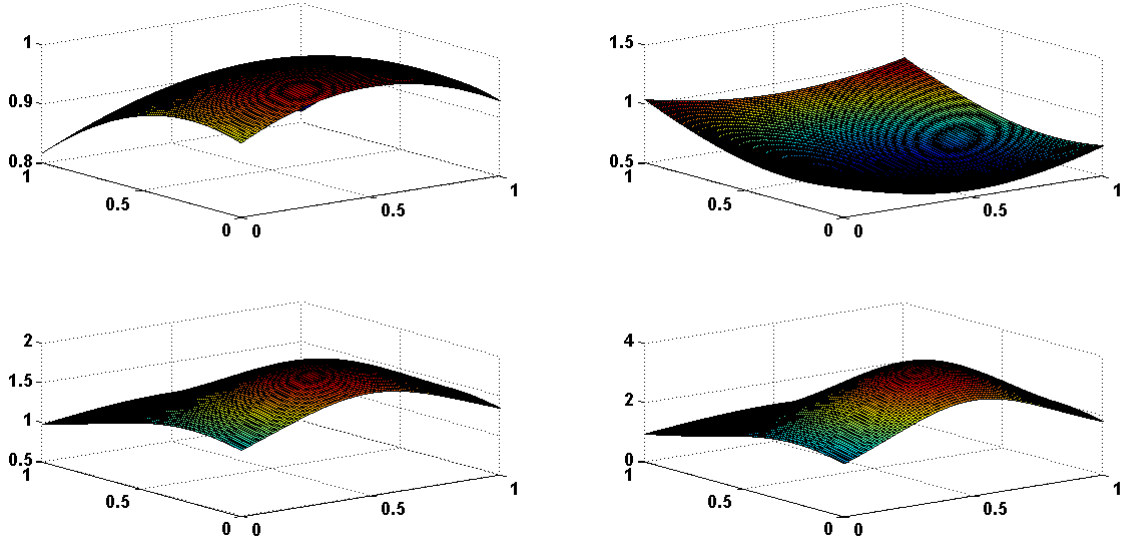


Figure 2.2: Gaussian RBF (left), Multiquadric (right), Inverse multiquadric (left), Quadric (right) for the center $(1/4, 1/2)$.

2.2 Interpolation by RBF

The theory of multivariable interpolation in high-dimensional space has a long history [15, 4].

Definition 2.3

Given a set of n distinct data points $\{x_j\}_{j=1}^n$ and corresponding data values $\{f_j\}_{j=1}^n$, the radial basis function interpolant is given by

$$s(x) = \sum_{j=1}^n \lambda_j \phi(\|x - x_j\|), \quad (2.11)$$

where $\phi(r), r \geq 0$, is some radial functions. The expansion coefficients λ_j are determined from the interpolation conditions

$$s(x_j) = f_j, j = 1, \dots, n, \quad (2.12)$$

which leads to the following symmetric linear system:

$$\begin{bmatrix} A \end{bmatrix} \begin{bmatrix} \lambda \end{bmatrix} = \begin{bmatrix} f \end{bmatrix},$$

where the entries of A are given by $a_{j,k} = \phi(\|x_j - x_k\|)$.

2.2.1 Multivariate Interpolation and Positive Definiteness

The simplest case of reconstruction of a d -variate unknown function f from data occurs when only a finite number of data in the form of values $f(x_1), \dots, f(x_m)$ at arbitrary locations

x_1, \dots, x_m in \mathbb{R}^d forming a set $X := \{x_1, \dots, x_m\}$ are known. To calculate a trial function f which reproduces the data $f(x_1), \dots, f(x_m)$ well, we have to solve the $m \times n$ linear system

$$\sum_{k=1}^n \alpha_k \phi(\|x_i - y_k\|_2) \approx f(x_i), 1 \leq i \leq m, \quad (2.13)$$

for the n coefficients $\alpha_1, \dots, \alpha_n$. The matrix with entries $\phi(\|x_i - y_k\|_2)$, is called "kernel matrices in machine learning". We can take $m \geq n$ or the centers y_k of trial functions are chosen to be identical to the data locations x_j for $1 \leq j \leq m = n$. By enforcing the exact interpolation conditions

$$f(x_j) = \sum_{k=1}^n \alpha_k \phi(\|x_j - x_k\|_2), 1 \leq j \leq m = n. \quad (2.14)$$

This is a system of m linear equations with unknowns $\alpha_1, \dots, \alpha_n$ with a symmetric coefficients matrix

$$A_X := (\phi(\|x_j - x_k\|_2))_{1 \leq j, k \leq m=n}. \quad (2.15)$$

In general, solvability of such a system is a serious problem.

Definition 2.4 *A radial basis function ϕ on $[0; \infty)$ is "positive definite" on \mathbb{R}^d , if for all choices of sets $\{X := x_1, \dots, x_m\}$ of finitely many points $x_1, \dots, x_m \in \mathbb{R}^d$ and arbitrary m the symmetric $m \times m$ symmetric matrices A_X of (2.15) are positive definite.*

2.2.2 Piecewise polynomial functions with local support

A compactly supported radial basis function are introduced first by Wu [18] and after by Wendland [15]. Several function spaces used for approximations possess locally supported basis functions. A local support of the basis function is only one step on the way to an efficient numerical approximation scheme. So, we are interested to functions of the form

$$\phi(r) = \begin{cases} p(r) & 0 \leq r \leq 1 \\ 0 & r > 1, \end{cases} \quad (2.16)$$

where p denotes a univariate polynomial. Of course, these functions are extended to the whole real line, again by even extension. We can restrict ourselves to functions with support in $[0, 1]$ or $[-1, 1]$, respectively. Other intervals can be obtained by scaling, because this does not change a function from being positive definite. The d -variate Fourier transform of $\phi(\cdot/\delta)$, $\delta > 0$, is $\delta^d (\mathcal{F}_d \phi)(\delta \cdot)$, which is nonnegative if and only if the Fourier transform of ϕ is nonnegative. The

function

$$\phi_l(r) = (1 - r)_+^l, \quad (2.17)$$

is positive definite on \mathbb{R}^d provided that $[l \geq [d/2] + 1]$.

These functions, when seen as even functions, are only continuous, even for large l . Since the basis function determines the smoothness of the approximant, it is necessary to have smoother functions of the form (2.16) as well. Numerical considerations, however, ask for a polynomial of the lowest possible degree. Hence it is quite natural to look for a function of the form (2.16) with a polynomial of minimal degree, if its smoothness and space dimension are prescribed. Some compactly supported radial basis functions are summarized in table (2.2)

Theorem 2.3 [16] *The functions $\phi_{d,k}$ are positive definite on \mathbb{R}^d and are of the form*

$$\phi_{d,k}(r) = \begin{cases} p_{d,k}(r) & 0 \leq r \leq 1, \\ 0 & r > 1, \end{cases}$$

with a univariate polynomial $p_{d,k}$ of degree $[d/2] + 3k + 1$. They possess continuous derivatives up to order $2k$. They are of minimal degree for given space dimension d and smoothness $2k$ and are up to a constant factor uniquely determined by this setting.

Space dimension	Function	Smoothness
$d = 1$	$\phi_{1,0}(r) = (1 - r)_+$	C^0
	$\phi_{1,1}(r) = (1 - r)_+^3(3r + 1)$	C^2
	$\phi_{1,2}(r) = (1 - r)_+^5(8r^2 + 5r + 1)$	C^4
$d \leq 3$	$\phi_{3,0}(r) = (1 - r)_+^2$	C^0
	$\phi_{3,1}(r) = (1 - r)_+^4(4r + 1)$	C^2
	$\phi_{3,2}(r) = (1 - r)_+^6(35r^2 + 18r + 3)$	C^4
$d \leq 5$	$\phi_{3,3}(r) = (1 - r)_+^8(32r^3 + 25r^2 + 8r + 1)$	C^6
	$\phi_{5,0}(r) = (1 - r)_+^3$	C^0
	$\phi_{5,1}(r) = (1 - r)_+^5(5r + 1)$	C^2
	$\phi_{5,2}(r) = (1 - r)_+^7(16r^2 + 7r + 1)$	C^4

Table 2.2: Compactly supported functions of minimal degree

2.2.3 Error estimate for RBFs

Here, we want to represent the error estimate of RBFs interpolation in terms of the fill distance parameter. All radial basis and strictly positive-definite functions give rise to reproducing kernels with respect to some Hilbert space which are named native Hilbert spaces.

Definition 2.5 Suppose $\phi \in C(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$ is a real-valued strictly positive definite function. Then the real native Hilbert space respect to reproducing kernel $\phi(\cdot - \cdot)$ is

$$\mathcal{N}_\phi(\mathbb{R}^d) = \left\{ f \in C(\mathbb{R}^d) \cap L^2(\mathbb{R}^d) : \frac{\hat{f}}{\sqrt{\hat{\phi}}} \in L^2(\mathbb{R}^d) \right\}. \quad (2.18)$$

with inner product

$$\langle f, g \rangle_{\mathcal{N}_\phi(\mathbb{R}^d)} = \frac{1}{\sqrt{2\pi}} \left\langle \frac{\hat{f}}{\sqrt{\hat{\phi}}}, \frac{\hat{g}}{\sqrt{\hat{\phi}}} \right\rangle_{L^2(\mathbb{R}^d)} = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}^d} \frac{\hat{f}(w)\overline{\hat{g}(w)}}{\sqrt{\hat{\phi}}} dw. \quad (2.19)$$

where \hat{f} denotes Fourier transform of f .

We concluded that the native spaces can be regarded as an extension of the standard Sobolev spaces. In other words, if the Fourier transform of strictly positive-definite function ϕ decays only algebraically, then the function ϕ has a corresponding Sobolev space as its native space. Now, we present some definitions, that are important to measure the quality of data points and to estimate the error of RBF interpolation method.

Definition 2.6 The fill distance of a set of points $X = \{x_1, \dots, x_N\} \subseteq D$ for a bounded domain D is defined by

$$h_{X,D} = \sup_{x \in D} \min_{0 \leq j \leq N} \|x - x_j\|_2.$$

Definition 2.7 The separation distance of $X = \{x_1, \dots, x_N\}$ is defined by

$$q_x = \frac{1}{2} \min_{i \neq j} \|x_i - x_j\|_2.$$

The set X is said to be quasi-uniform with respect to a constant $c > 0$ if $q_x \leq h_{X,D} \leq cq_x$.

Now, we give the convergence theorem for approximating a function $u \in \mathcal{N}_\phi(D)$ by the strictly positive-definite function. Before that we define the interior cone condition as follows:

Definition 2.8 A set $D \subset \mathbb{R}^d$ is said to satisfy an interior cone condition if there exists an angle $\theta \in (0, \pi/2)$ and a radius $r > 0$ such that for every $x \in D$ a unit vector $\xi(x)$ exists such that the cone

$$C(x, \xi(x), \theta, r) = \left\{ x + \lambda y : y \in \mathbb{R}^d, \|y\|_2 = 1, y^T \xi(x) \geq \cos \theta, \lambda \in [0, r] \right\}, \quad (2.20)$$

is contained in D .

Theorem 2.4 [16] Let ϕ be positive-definite RBF with infinitely smoothness. Suppose that $D \subset \mathbb{R}^d$ is open and bounded, satisfying an interior cone condition. Denote the interpolant of a

function $u \in \mathcal{N}_\phi(D)$ based on the RBF ϕ and the distinct set $X = \{x_1, \dots, x_N\}$ by $\mathcal{P}_N u$. Then for every $l \in \mathbb{N}$ there exist constants $h_0(l)$ and C_l such that

$$\|u - \mathcal{P}_n u\|_{L^\infty(D)} \leq C_l h_{X,D}^l |u|_{\mathcal{N}_\phi(D)}, \quad (2.21)$$

for all $x \in D$, provided $h_{X,D} \leq h_0(l)$.

Remark 2.1 As a conclusion from theorem 2.4, for the sufficiently small $h_{X,D}$, some positive constant c and $u \in \mathcal{N}_\phi(D)$, we list the error bound as follows:

For Gaussians $\phi(x) = \exp(-\alpha\|x\|^2)$, $\alpha > 0$, we have

$$\|u - P_N u\|_{L^\infty(D)} \leq \exp\left(\frac{-c|\log h_{X,D}|}{h_{X,D}}\right) |u|_{\mathcal{N}_\phi(D)}. \quad (2.22)$$

For inverse multiquadrics

$$\phi(x) = (\|x\|_2 + \alpha^2)^\beta, \alpha > 0, \beta < 0, \text{ or } \beta > 0 \text{ and } \beta \neq \mathbb{N},$$

we have

$$\|u - P_N u\|_{L^\infty(D)} \leq \exp\left(\frac{-c}{h_{X,D}}\right) |u|_{\mathcal{N}_\phi(D)}. \quad (2.23)$$

Therefore the convergence rates will be arbitrarily high algebraic for infinitely smooth RBFs such as GAs, MQs and IMQs and for RBFs with limited smoothness, the approximation order of the method is limited by the degree of smoothness.

Chapter 3

Some numerical treatment on the interpolation by RBF

This chapter is divided in two parts, in the first part, we use radial basis functions for solving Volterra-Fredholm integral equations, such equations have numerous applications in many problems in the applied sciences to model dynamical systems. The RBFs can be of various types, for example: polynomials of any chosen degree such as linear, cubic, thin plate spline (TPS), multiquadrics (MQ), inverse multiquadrics (IMQ), Gaussian forms (GA), hyperbolic secant (sech) form etc. In the cases of inverse quadratic, inverse multiquadric (IMQ), hyperbolic secant (sech) and Gaussian (GA), the coefficient matrix of RBFs interpolating is positive definite. A numerical technique based on the spectral method is presented for the solution of linear and nonlinear Volterra-Fredholm-Hammerstein (VFH) integral equations and by using zeros of the shifted Legendre polynomial as the collocation points, different applications of RBFs are used for this purpose. The integral involved in the formulation of the problem is approximated by Legendre-Gauss-Lobatto integration rule. Different choices of the shape parameter are given randomly, because the optimal choice of shape parameter is an open problem which is still under intensive investigation. In general, as the value of the shape parameter c increases, the matrix of the system to be solved becomes highly ill-conditioned and hence the condition number can be used in determining the critical value of the shape parameter for an accurate solution. Some numerical test are given to describe this problem. In the second parts, we present some numerical treatment of the condition number which can be used to some theoretical effort to bound the condition number of the interpolation matrix.

3.1 Some application of RBF for solving VFH

Consider the nonlinear Volterra–Fredholm–Hammerstein integral equations

$$y(x) = f(x) + \lambda_1 \int_0^x K_1(x, t)G_1(t, y(t))dt + \lambda_2 \int_0^1 K_2(x, t)G_2(t, y(t))dt \quad 0 \leq x \leq 1, \quad (3.1)$$

where λ_1 and λ_2 are constants, $f(x)$ and the kernels $G_1(x, t)$ and $G_2(x, t)$ are given functions for $0 \leq x \leq 1$ and $0 \leq t \leq 1$. In order to solve (3.1), we use a spectral method based on radial basis functions and the Gauss–Legendre rules to approximate the integrals.

3.1.1 Legendre–Gauss–Lobatto nodes and weights

Let $\mathcal{H}_N[-1, 1]$ denote the space of algebraic polynomials of degree $\leq N$. Let $\langle \cdot, \cdot \rangle$ represents the usual $L^2[-1, 1]$ inner product and $\{P_i\}_{i \geq 0}$ are the well-known Legendre polynomials of order i which are orthogonal with respect to the weight function $w(x) = 1$ on the interval $[-1, 1]$, and satisfy the following formula,

1. $\langle P_i, P_j \rangle = \frac{2}{2j+1} \delta_{ij}$,
2. $P_0(x) = 1 \quad P_1(x) = x$,
3. $P_{i+1}(x) = \left(\frac{2i+1}{i+1}\right)xP_i(x) - \left(\frac{i}{i+1}\right)P_{i-1}(x) \quad i = 1, 2, 3, \dots$

Let $\{x_j\}_{j=0}^N$ the points such that

$$(1 - x_j^2)P'(x_j) = 0,$$

$$-1 = x_0 < x_1 < x_2 < \dots < x_N = 1,$$

where $P'(x)$ is the derivative of $P(x)$. The points $\{x_j\}_{j=0}^N$ can be computed numerically [12]. Assume that $f \in \mathcal{H}_{2N-1}[-1, 1]$, we have

$$\int_{-1}^1 f(x)dx \approx \sum_{j=0}^N \omega_j f(x_j) = I_G(f), \quad (3.2)$$

where ω_j are the Legendre–Gauss–Lobatto weights given by

$$\omega_j = \frac{2}{N(N+1)} \times \frac{1}{(P_N(x_j))^2}. \quad (3.3)$$

3.1.2 Numerical technique for solving VFH integral equation

In order to get a numerical approximation of the solution of equation (3.1) by radial basis functions, we first approximate $y(x)$ as

$$y(x) \approx y_N(x) = \sum_{i=1}^{N+1} c_i \phi_i(x) = \Phi^T(x)C, \quad (3.4)$$

where $\Phi^T(x) = [\phi_1(x), \phi_2(x), \dots, \phi_{N+1}(x)]^t$ and $C = [c_1, c_2, \dots, c_{N+1}]^t$. Then, substituting equation (3.4) into equation (3.1), we get

$$\Phi^T(x)C = f(x) + \lambda_1 \int_0^x K_1(x, t)G_1(t, \Phi^T(t)C)dt + \lambda_2 \int_0^1 K_2(x, t)G_2(t, \Phi^T(t)C)dt. \quad (3.5)$$

We collocate equation (3.5) at points $\{x_i\}_{i=1}^N$, we have

$$\Phi^T(x_i)C = f(x_i) + \lambda_1 \int_0^{x_i} K_1(x_i, t)G_1(t, \Phi^T(t)C)dt + \lambda_2 \int_0^1 K_2(x_i, t)G_2(t, \Phi^T(t)C)dt. \quad (3.6)$$

In order to use the Legendre–Gauss–Lobatto integration on the interval $[-1, 1]$, we use the change of variables $\sigma_1 = \frac{2}{x_i}t - 1$, $\sigma_2 = 2t - 1$, then, the intervals $[0, x_i]$ and $[0, 1]$ are transformed to the interval $[-1, 1]$, respectively. Let

$$H_1(x_i, t) = K_1(x_i, t)G_1(t, \Phi^T(t)C), \quad H_2(x_i, t) = K_2(x_i, t)G_2(t, \Phi^T(t)C), \quad (3.7)$$

then, equation (3.6) may then be restated as

$$\Phi^T(x_i)C = f(x_i) + \lambda_1 \frac{x_i}{2} \int_{-1}^1 H_1(x_i, \frac{x_i}{2}(\sigma_1 + 1))d\sigma_1 + \frac{\lambda_2}{2} \int_{-1}^1 H_2(x_i, \frac{1}{2}(\sigma_2 + 1))d\sigma_2, \quad (3.8)$$

to approximate the integrals appeared in equation (3.8), we use Legendre–Gauss–Lobatto integration formula. Then the corresponding residual function $Res(x)$ is given by

$$Res(x_i) = -\Phi^T(x_i)C + f(x_i) + \lambda_1 \frac{x_i}{2} \sum_{j=0}^{r1} W_{1j} H_1(x_i, \frac{x_i}{2}(\sigma_{1j} + 1)) + \frac{\lambda_2}{2} \sum_{j=0}^{r2} W_{2j} H_2(x_i, \frac{1}{2}(\sigma_{2j} + 1)), \quad (3.9)$$

for $i = 1 \dots N + 1$. Equation (3.9) generates an $N + 1$ set of nonlinear equations which can be solved by iterative method for the unknown C .

3.1.3 Numerical tests

This section investigates the obtained results of the presented approach on some test problems. The error norms and condition numbers are computed.

Example 3.1

Consider the following Hammerstein integral equation [12].

$$y(x) = e^x - \frac{1}{3}e^{3x} + \frac{1}{3} + \int_0^x y^3(t)dt, \quad (3.10)$$

with the exact solution

$$y(x) = e^x.$$

We solve equation (3.10) with different values of N . Table (3.1) and (3.2) shows the absolute error between the exact solution and different RBFs approximations, for $\epsilon = 1.8$

x	N = 6			N = 4		
	IMQ	MQ	GA	IMQ	MQ	GA
0	2.5757e-14	5.6843e-14	1.3531e-16	8.8818e-15	9.0949e-13	3.4694e-18
0.1	1.6043e-4	6.9611e-5	1.5628e-3	2.9712e-3	6.4130e-1	1.6402e-2
0.2	7.1137e-5	2.5950e-5	1.0591e-3	4.4858e-3	1.4081	2.8516e-2
0.3	6.7777e-4	2.6953e-4	8.5471e-3	3.4612e-3	2.1824	2.5491e-2
0.4	1.2932e-3	5.1070e-4	1.6536e-2	4.6833e-4	2.8228	1.2730e-3
0.5	1.3204e-3	5.1786e-4	1.6886e-2	6.4655e-3	3.1802	3.9247e-2
0.6	3.2382e-4	1.2618e-4	3.8582e-3	1.2101e-2	3.1146	7.6842e-2
0.7	1.3480e-3	5.2868e-4	1.6876e-2	1.3147e-2	2.5101	7.9285e-2
0.8	1.8521e-3	7.2899e-4	2.1406e-2	3.6037e-3	1.2864	7.6792e-3
0.9	2.7464e-3	1.0994e-3	3.1824e-2	2.4031e-2	5.9554e-1	1.7389e-1
1	1.8770e-2	7.5968e-3	1.9207e-1	7.8306e-2	3.1322	4.8857e-1
$cond_2$	2.5823e+5	2.1109e+6	1.0153e+002	3.7264e+3	1.9497e+4	6.9461
$cond_\infty$	3.1932e+5	2.4581e+6	1.3916e+002	4.5170e+3	2.3943e+4	8.2390

Table 3.1: Comparison between exact and approximate solutions for different values of N .

Example 3.2 Consider the nonlinear Volterra–Fredholm–Hammerstein integral equation of the form [12].

$$y(x) = g(x) + \int_0^x (x-t)y^2(t)dt + \int_0^1 (x+t)y(t)dt, \quad (3.11)$$

where

$$g(x) = \frac{1}{30}x^6 + \frac{1}{3}x^4 - x^2 + \frac{5}{3}x - \frac{5}{4}, \quad (3.12)$$

which has the exact solution $y(x) = x^2 - 2$. We applied the RBFs approach to solve equation (3.11), for $\epsilon = 0.2$. The numerical results are represented in table (3.3) and (3.4).

x	N = 6			N = 4		
	IMQ	MQ	GA	IMQ	MQ	GA
x_1	$1.9583e - 14$	$4.3422e - 22$	$4.4109e - 17$	$1.7020e - 23$	$1.3126e - 23$	$1.0591e - 16$
x_2	0.0013204	$5.1786e - 4$	0.016886	$6.4655e - 3$	3.1802	0.039247
x_3	0.0042477	$1.7015e - 3$	0.04799	$1.8059e - 3$	$8.3808e - 001$	0.02974
x_4	0.001804	$7.0817e - 4$	0.022056	$4.2873e - 3$	1.1923	0.026283
x_5	0.00015754	$6.8414e - 5$	0.0015264	$7.8306e - 2$	3.1322	0.48857
x_6	0.00044228	$1.7573e - 4$	0.0055791			
x_7	0.01877	$7.5968e - 3$	0.19207			
$L_2(norm)$	1.9380e-2	7.8366e-3	1.9999e-1	7.8710e-2	4.6955	4.9175e-1
$L_\infty(norm)$	1.8770e-2	7.5968e-3	1.9207e-1	7.8306e-2	3.1802	4.8857e-1

Table 3.2: Comparison between exact and approximate solutions at collocation points for different values of N .

x	N=3	
	IMQ	MQ
0	6.2263e-001	1.8764e+000
0.1	5.8198e-001	2.2178e+000
0.2	4.4076e-001	2.5472e+000
0.3	1.9596e-001	2.8726e+000
0.4	7.5512e-002	3.2113e+000
0.5	1.5195e-001	3.5848e+000
0.6	4.6589e-002	3.9893e+000
0.7	1.6778e-002	4.3958e+000
0.8	3.4032e-002	4.7744e+000
0.9	1.8041e-001	5.0906e+000
1	3.3271e-001	5.2932e+000
$cond_2$	2.6054e+000	1.6234e+001
$cond_\infty$	3.0314e+000	2.1376e+001

Table 3.3: Comparison between exact and approximate solutions for different values of x for $N = 3$.

x	N=3	
	IMQ	MQ
x_1	$6.2263e - 001$	1.8764
x_2	$1.5243e - 002$	4.4887
x_3	2.6168	2.7954
x_4	$3.3271e - 001$	5.2932
$L_2(norm)$	7.5304e-001	7.7138e+000
$L_\infty(norm)$	6.2263e-001	5.2932e+000

Table 3.4: Comparison between exact and approximate solutions at collocation points for $N = 3$.

Example 3.3

Let given the nonlinear Volterra-Hammerstein integral equation

$$y(x) = \sin(\pi x) + \int_0^1 \sin(\pi t) \cos(\pi x) y^3(t) dt, \quad (3.13)$$

where the exact solution is given by

$$y(x) = \sin(\pi x) + \frac{20 - \sqrt{391}}{3} \cos(\pi x) \quad x \in [0, 1]. \quad (3.14)$$

We take $\epsilon = 1$. The numerical results are summarized in tables (3.5) and (3.6).

	N=8		
x	IMQ	MQ	GA
0	4.2013e-005	9.1202e-005	1.3118e-005
0.1	1.1104e-003	1.4392e-003	2.1034e-004
0.2	1.3670e-003	1.9115e-003	2.7602e-004
0.3	6.5179e-004	9.7613e-004	1.4000e-004
0.4	3.7246e-004	6.2169e-004	8.9210e-005
0.5	8.5551e-004	1.5576e-003	2.2547e-004
0.6	5.0241e-004	1.0341e-003	1.5270e-004
0.7	1.5268e-004	3.6455e-004	5.5021e-005
0.8	3.4254e-004	1.0142e-003	1.5991e-004
0.9	3.9223e-005	8.3622e-005	1.1954e-005
1	4.2013e-005	9.1202e-005	1.3118e-005
$cond_2$	6.7171e+004	6.8750e+005	4.1378e+006
$cond_\infty$	1.0022e+005	1.0140e+006	5.5492e+006

Table 3.5: Comparison between exact and approximate solutions at different points x for $N = 8$.

	N=8		
x	IMQ	MQ	GA
x_1	0.000042013	0.000091202	0.000013118
x_2	0.00085551	0.0015576	0.00022547
x_3	0.000046278	0.00037908	0.000068128
x_4	0.00061016	0.00074759	0.00011022
x_5	0.00024936	0.00080444	0.0001288
x_6	0.000048997	0.00011102	0.000016421
x_7	0.0013981	0.0019012	0.00027565
x_8	0.00045883	0.00069411	0.000099493
x_9	0.000042013	0.000091202	0.000013118
$L_2(norm)$	1.8274e-003	2.8109e-003	4.1317e-004
$L_\infty(norm)$	1.3981e-003	1.9012e-003	2.7565e-004

Table 3.6: Comparison between exact and approximate solutions at collocation points for $N = 8$.

Example 3.4 Let consider the linear integral equation

$$y(x) = \cos x - \sin x \exp(x) + \int_0^x \exp(x)y(t)dt \quad x \in [0, 1]. \quad (3.15)$$

The exact solution is given by

$$y(x) = \cos x.$$

We take $\epsilon = 0.2$. The obtained numerical results are presented in tables (3.7) and (3.8).

	N=5		
x	IMQ	MQ	GA
0	0.1872	0.0145	6.6321e-006
0.1	0.1631	0.0134	6.3520e-006
0.2	0.0872	0.0085	4.4467e-006
0.3	0.0494	0.0035	1.5250e-006
0.4	0.1133	0.0008	1.4584e-006
0.5	0.1859	0.0014	3.4142e-006
0.6	0.2097	0.0036	3.4169e-006
0.7	0.2114	0.0014	1.0899e-006
0.8	0.2905	0.0123	2.9286e-006
0.9	0.4708	0.0301	6.4428e-006
1	0.5912	0.0227	5.0853e-006
$cond_2$	7.0106	8.1566e+001	1.1176e+010
$cond_\infty$	8.5266	1.1793e+002	1.3622e+010

Table 3.7: Comparison between exact and approximate solutions at different points x for $N = 5$.

	N=5		
x	IMQ	MQ	GA
x_1	0.18722	0.014531	6.6321e - 006
x_2	0.20872	0.0037066	6.024e - 006
x_3	0.43783	0.027825	2.7019e - 006
x_4	0.078168	0.0017566	6.1246e - 006
x_5	0.15224	0.012709	2.4933e - 007
x_6	0.59116	0.022695	5.0853e - 006
$L_2(norm)$	0.8057	0.0410	1.2288e-005
$L_\infty(norm)$	0.5912	0.0278	6.6321e-006

Table 3.8: Comparison between exact and approximate solutions at collocation points for $N = 5$.

From, the previous tests and through the comparison with exact solutions we show that the RBFs methods have good reliability and efficiency. Also, we can see that the accuracy depend on the choose of radial basis functions and the shape parameter. We can remark also in some examples the ill-conditioned problems and the independence between the accuracy and the condition number.

3.2 Numerical test of condition number by RBF

One of the serious problems is that when the RBFs are wide compared to the average grid spacing h , the RBF interpolation matrix is very ill-conditioned. This is very unfortunate because it is known that RBF accuracy generally increases in the “flat” limit and is unreservedly awful in the opposite limit of RBFs. This has inspired some theoretical effort to bound the condition number of the interpolation matrix. However, it is very difficult to obtain sharp bounds and the estimates cataloged in "Wendland's book [16]" are wildly pessimistic, at least for a uniform grid. Through some numerical tests, we examine the condition numbers of the interpolation matrix for some kind of RBF, we give some relation between the condition number and the shape parameter and if it depend on the number N of interpolation points. The shape parameter ε is the “absolute inverse width”, a user-choosable parameter often replaced in applications by the “relative inverse width” α where $\varepsilon = \alpha/h$ with h as the average grid spacing, for this a radial basis function can be written in the following form

$$f(x) \approx f^{RBF}(x, N) = \sum_{j=1}^N \lambda_j \phi([\alpha/h] \|x - x_j\|_2), x \in \mathbb{R}^d, \quad (3.16)$$

for some function $\phi(r)$ and some set of N points x_j , which are called the “centers”. Here h is the grid spacing (for a uniform grid) or the average grid spacing (for a non-uniform grid) and α is the “relative inverse width parameter”. Many species of $\phi(r)$. The RBF coefficients λ_j are usually found by interpolation at a set of points y_k that may or may not coincide with the centers. The interpolation condition is

$$f(x_j) = f^{RBF}(x_j, N), j = 1, 2, \dots, N. \quad (3.17)$$

These can be organized into a matrix system. The interpolation matrix, which is also known as the “generalized Vandermonde matrix”, is a symmetric matrix (for coincident centers and interpolation points) with the elements

$$A_{ij} = \phi([\alpha/h] \|x_i - x_j\|_2). \quad (3.18)$$

On a uniform grid with spacing h , the elements of the interpolation matrix are independent of h and depend only on α :

$$A_{ij} = \phi(\alpha \|S_i - S_j\|_2), \quad (3.19)$$

where the $S_i = x_i/h$ are the points on a grid rescaled to have unit grid spacing. Consequently, the condition number of the matrix is a function only of N , the size of the matrix, and of α .

The condition number $\kappa(\alpha, N)$ is given by

$$\kappa = \|A\|_{\infty} \|A^{-1}\|_{\infty}. \quad (3.20)$$

We can analysis the problem of condition number in some steps. First, we plotted the condition number versus N for several α . Secondly, we graphed the condition number for a fixed large N versus α and versus α^2 . All these steps are done for some radial basis functions such that Gaussian, multiquadric and inverse multiquadric. For radial basis function methods, it is far better to choose sufficiently large α so that the condition number is not too a big.

The following program indicate the relation between the number N of interpolation points and condition number.

Program

- *Digits* = 25;
- alpha=1 ; ncase=100;
- C=[]; d=[];
- for j=1:ncase
- N=2+2*(j-1); h=2/(N-1); epsilon=(alpha/h);
- xgrid=zeros(N,1);
- d=[d;N]
- for j = 1:1: N
- xgrid(j)=-1+2*(j-1)/(N-1);
- end
- G=zeros(N,N);
- for i=1:N
- for j=1:N
- $rsq = (xgrid(i) - xgrid(j))^2$;
- $G(i, j) = (1/sqrt(1 + (epsilon)^2 * rsq))$;

- end
- end
- C=[C; norm(G,inf)*norm(inv(G), inf)];
- end
- plot(d, C)

3.2.1 Multiquadrics (MQ) on one dimension

For this radial basis function, it can be shown that the condition number for fixed α grows quadratically with the number of points N , which can be seen in figures (3.4)-(3.7) and approximately, we have

$$\kappa(\alpha, N) = 0.363N^2 \exp(3.07/\alpha) \quad [1]. \quad (3.21)$$

The plot of this function is given in figure (3.17) and has approximately the same plot with the figure (3.18). Table (3.9) show that the condition number is independent of matrix size N for large N .

Multiquadric				
N	$\alpha = 1/8$	$\alpha = 1/4$	$\alpha = 1/2$	$\alpha = 1$
2000	5.3684e+016	2.1504e+011	5.5290e+008	3.2172e+007
2002	5.2154e+016	2.1547e+011	5.5401e+008	3.2236e+007
2004	5.2683e+016	2.1590e+011	5.5512e+008	3.2300e+007
2006	5.4672e+016	2.1633e+011	5.5623e+008	3.2365e+007
2008	5.2861e+016	2.1677e+011	5.5734e+008	3.2429e+007
2010	5.2889e+016	2.1720e+011	5.5845e+008	3.2494e+007
2012	5.3862e+016	2.1763e+011	5.5956e+008	3.2559e+007
2014	5.3816e+016	2.1806e+011	5.6067e+008	3.2624e+007
2016	5.4317e+016	2.1850e+011	5.6179e+008	3.2688e+007
2018	5.2739e+016	2.1893e+011	5.6290e+008	3.2753e+007

Table 3.9: Condition number versus N for different values of alpha for multiquadric.

3.2.2 Gaussian RBFs on one-dimension with uniform grid

On a uniform one-dimensional grid of spacing h , Gaussian RBFs are of the form

$$\Phi(x, \alpha, h) = \exp(-[\alpha^2/h^2]x^2). \quad (3.22)$$

We can normalize the interpolation interval to $x \in [-1, 1]$ without loss of generality, the uniform grid spacing is $h = 2/(N - 1)$ and the grid points $x_j = -1 + (j - 1)h$. The elements of the interpolation matrix are

$$A_{ij}(\alpha) = \exp(-\alpha^2(i - j)^2). \quad (3.23)$$

We analyzed the condition number in two stages.

- First, we graphed $\kappa(\alpha, N)$ versus N for several α . This showed that the condition number is independent of matrix size N for large N as illustrated in figures(3.8)-(3.10) and table (3.10).
- Secondly, we plotted the condition number for a fixed large N versus α^2 , as presented in figure(3.12).

Some numerical tests gives the analytic approximation [1],

$$\kappa_{anal}^{Gauss}(\alpha) = (1/2) \exp(\pi^2/(4\alpha^2)), \quad (3.24)$$

and this is represented in figure (3.15)and it is similar to figure (3.12). Because this formula was derived by numerical experimentation and not a deductive proof, we shall regard the statement

$$\lim_{N \rightarrow \infty} \kappa(\alpha) = \kappa_{anal}^{Gauss}(\alpha). \quad (3.25)$$

is a highly probable conjecture.

Gaussian				
N	$\alpha = 1/8$	$\alpha = 1/4$	$\alpha = 1/2$	$\alpha = 1$
2000	7.7592e+018	3.1075e+018	9.6664e+003	5.8965e+000
2002	1.8057e+019	5.5745e+018	9.6664e+003	5.8965e+000
2004	1.4973e+019	4.8513e+017	9.6664e+003	5.8965e+000
2006	2.5782e+019	3.2542e+016	9.6664e+003	5.8965e+000
2008	1.0722e+020	1.7157e+018	9.6664e+003	5.8965e+000
2010	3.3639e+019	5.1259e+018	9.6664e+003	5.8965e+000
2012	9.7390e+019	1.8654e+019	9.6664e+003	5.8965e+000
2014	7.8975e+018	7.3806e+018	9.6664e+003	5.8965e+000
2016	1.6104e+019	3.2207e+019	9.6664e+003	5.8965e+000
2018	2.8240e+020	5.2742e+018	9.6664e+003	5.8965e+000

Table 3.10: Condition number versus N for different values of alpha for gaussian.

3.2.3 Inverse quadratics on one dimension

Inverse multiquadric RBFs is defined by

$$\phi(r, \alpha, h) = \frac{1}{1 + [\alpha/h]^2 r^2}. \quad (3.26)$$

Like Gaussians, inverse quadratic RBFs can yield an exponential rate of convergence if the function $f(x)$ being approximated is analytic on the approximation interval. The condition number $\kappa(N)$ asymptotes to an α -dependent number as $N \rightarrow \infty$ for fixed α . The figures (3.1)- (3.3) shows the plot of condition number versus N for different values of α . Figures (3.11)-(3.19) shows the plot of the condition number versus α for $N = 200$. The plot of the condition number versus α^2 is represented in figure (3.14). It is known that the saturation error for IQ functions is proportional to $\exp(-\pi/\alpha)$, but the numerical results suggested that the asymptote is roughly [1]

$$\kappa_{anal}^{IQ}(\alpha) = (1/2) \exp(\pi/\alpha). \quad (3.27)$$

The figures(3.16) gives the plot of this function, and it is similar to the figure (3.19) for inverse multiquadric condition number. When we plotted the difference between $\kappa(N, \alpha)$ and $\kappa_{anal}^{IQ}(\alpha)$ on both log-linear and log-log axes, we found the curves on the log-linear scale became flatter as N increased whereas the difference curves were nearly linear on the log-log plate. This implies that the IQ conditions are not asymptoting exponentially as true of Gaussians but rather as $1/N$. Some numerical tests are summarized in table (3.11), and it showed that the condition number is independent of N with N sufficiently large. Some good numerical results given by some researchers are collected in table (3.12) for different radial basis functions [1].

Inverse multiquadric				
N	$\alpha = 1/8$	$\alpha = 1/4$	$\alpha = 1/2$	$\alpha = 1$
2000	8.7400e+011	2.4491e+006	3.6411e+003	1.2473e+002
2002	8.7416e+011	2.4495e+006	3.6416e+003	1.2475e+002
2004	8.7433e+011	2.4499e+006	3.6421e+003	1.2477e+002
2006	8.7449e+011	2.4503e+006	3.6427e+003	1.2478e+002
2008	8.7466e+011	2.4507e+006	3.6432e+003	1.2480e+002
2010	8.7483e+011	2.4511e+006	3.6438e+003	1.2482e+002
2012	8.7499e+011	2.4515e+006	3.6443e+003	1.2484e+002
2014	8.7515e+011	2.4519e+006	3.6449e+003	1.2485e+002
2016	8.7531e+011	2.4523e+006	3.6454e+003	1.2487e+002
2018	8.7548e+011	2.4527e+006	3.6459e+003	1.2489e+002

Table 3.11: Condition number versus N for different values of alpha for inverse multiquadric.

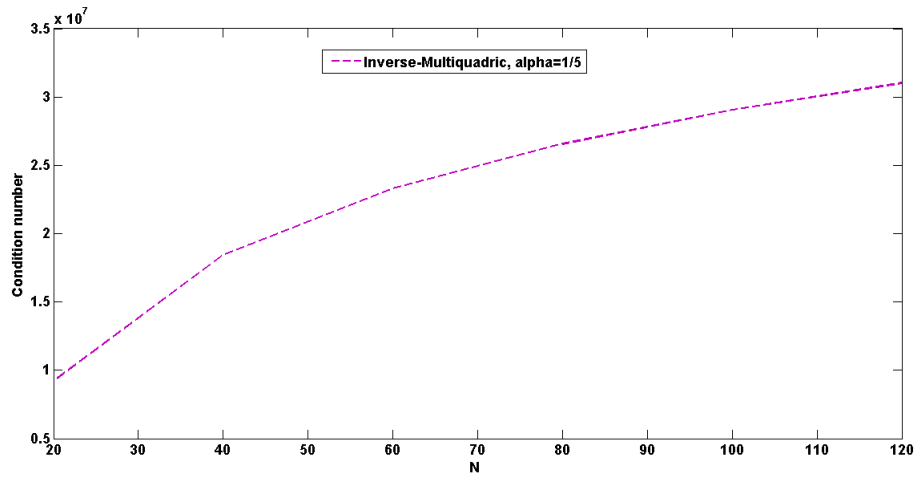


Figure 3.1: The matrix condition number for the interpolation Matrix of IMQ RBF on one dimensional uniforme grid.

Name	κ
Gaussian 1D	$(1/2) \exp(\pi^2/[4\alpha^2])$
Gaussian 2D	$(1/4) \exp(\pi^2/[2\alpha^2])$
sech 1D	$(1/4) \exp(\pi^2/(2\alpha))$
sech 2D	$0.26 \exp(7.20/\alpha)$
IQ 1D	$(1/2) \exp(\pi/\alpha)$
MQ 1D	$0.363N^2 \exp(3.07/\alpha)$
Cubic MN3	$(2\sqrt{3} - 3)N^5$
Quintic MN5	$0.112322124N^8$
Thin-plate splines TPS2	$0.1198139997N^4$
Thin-plate splines TPS4 ($r^4 \log(r)$)	$0.05304350371N^7$

Table 3.12: Condition number: uniform grid.

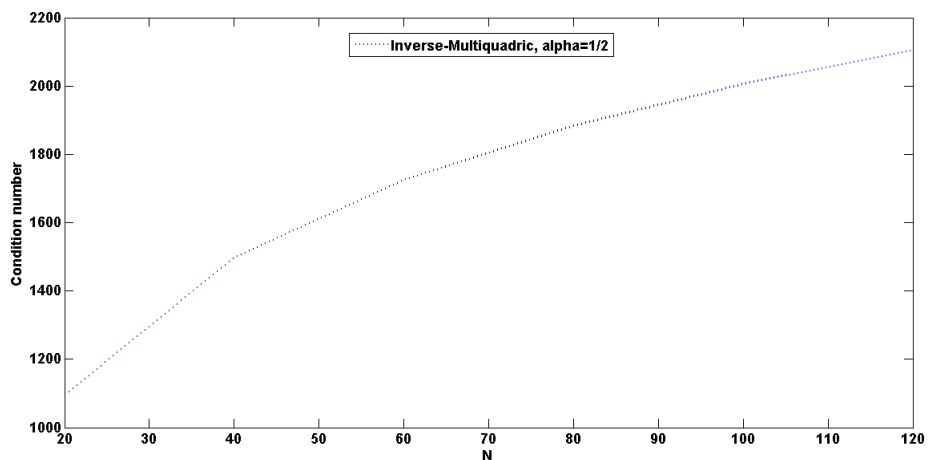


Figure 3.2: The matrix condition number for the interpolation Matrix of IMQ RBF on one dimensional uniforme grid.

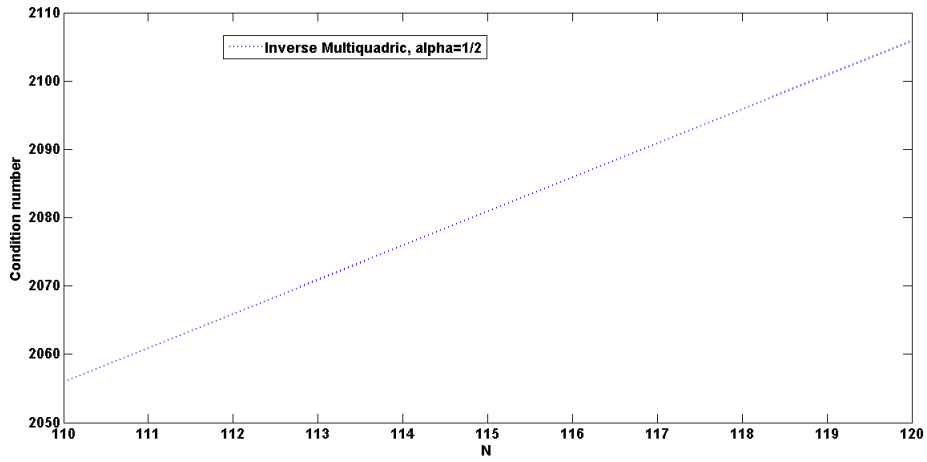


Figure 3.3: The matrix condition number for the interpolation Matrix of IMQ RBF on one dimensional uniforme grid.

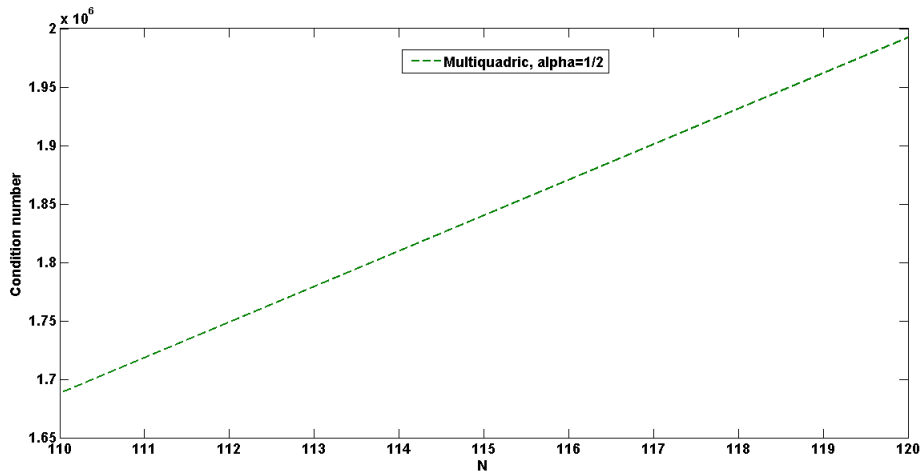


Figure 3.4: The matrix condition number for the interpolation Matrix of MQ RBF on one dimensional uniforme grid.

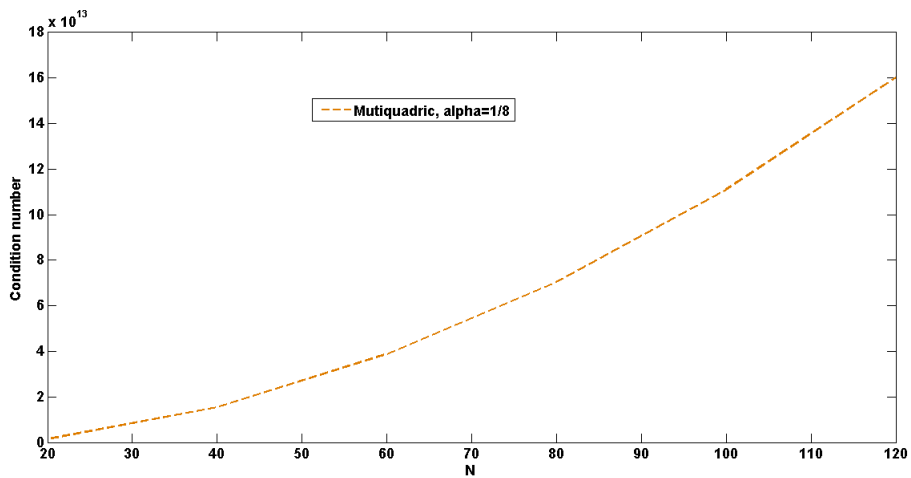


Figure 3.5: The matrix condition number for the interpolation Matrix of MQ RBF on one dimensional uniforme grid.

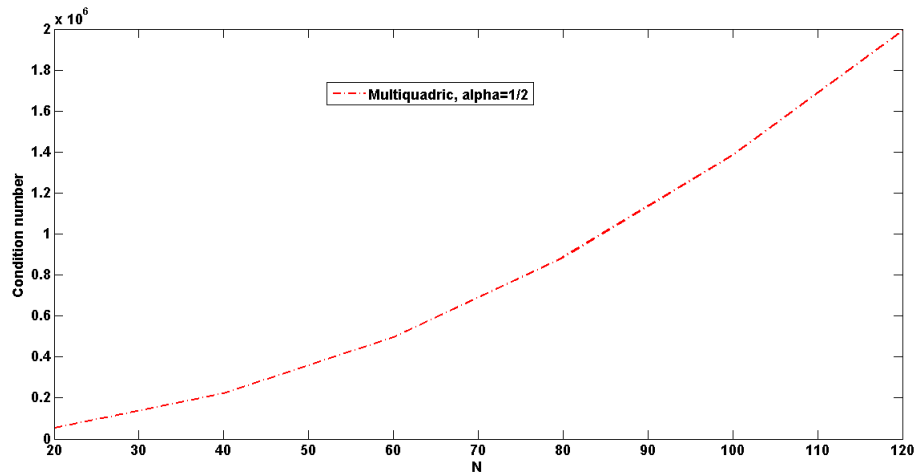


Figure 3.6: The matrix condition number for the interpolation Matrix of MQ RBF on one dimensional uniforme grid.

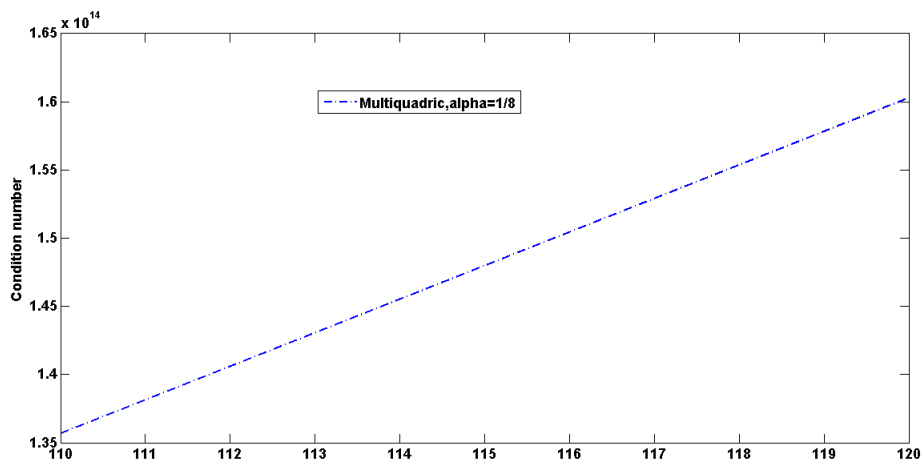


Figure 3.7: The matrix condition number for the interpolation Matrix of MQ RBF on one dimensional uniforme grid.

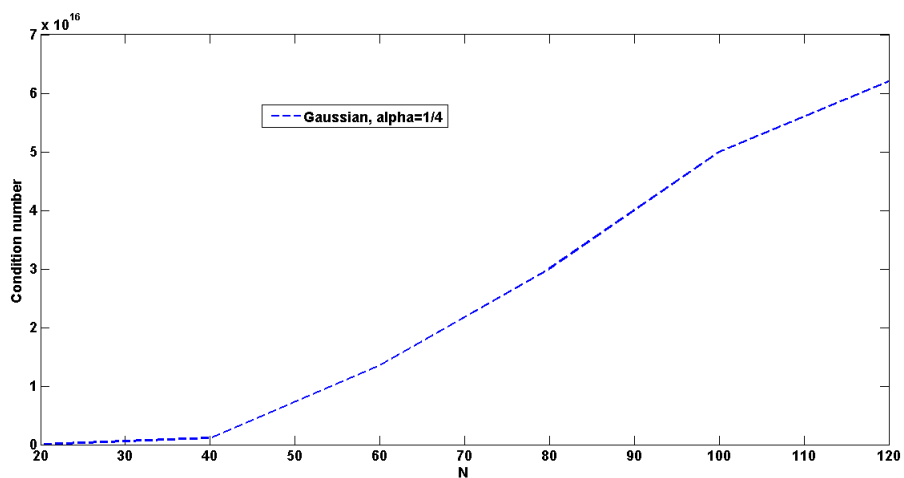


Figure 3.8: The matrix condition number for the interpolation Matrix of Gaussian RBF on one dimensional uniforme grid.

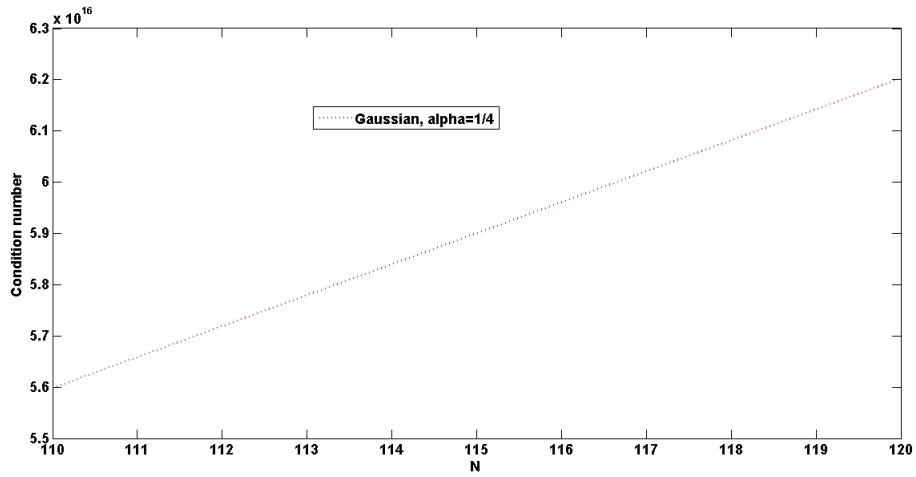


Figure 3.9: The matrix condition number for the interpolation Matrix of Gaussian RBF on one dimensional uniform grid.

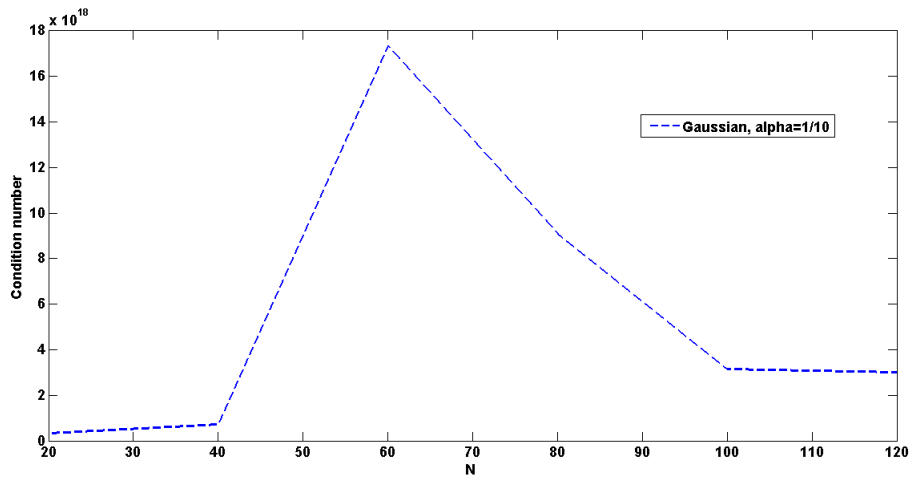


Figure 3.10: The matrix condition number for the interpolation Matrix of Gaussian RBF on one dimensional uniform grid.

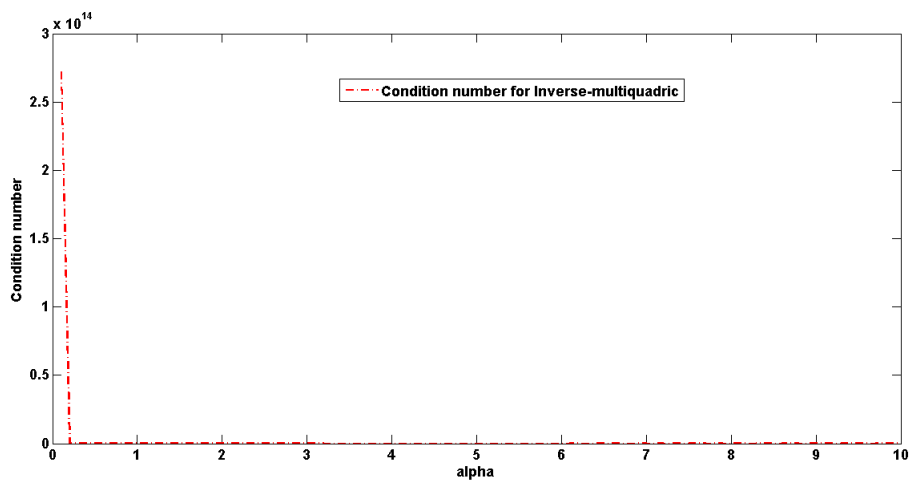


Figure 3.11: Condition number of IMQ RBFs for different values of alpha for $N = 200$.

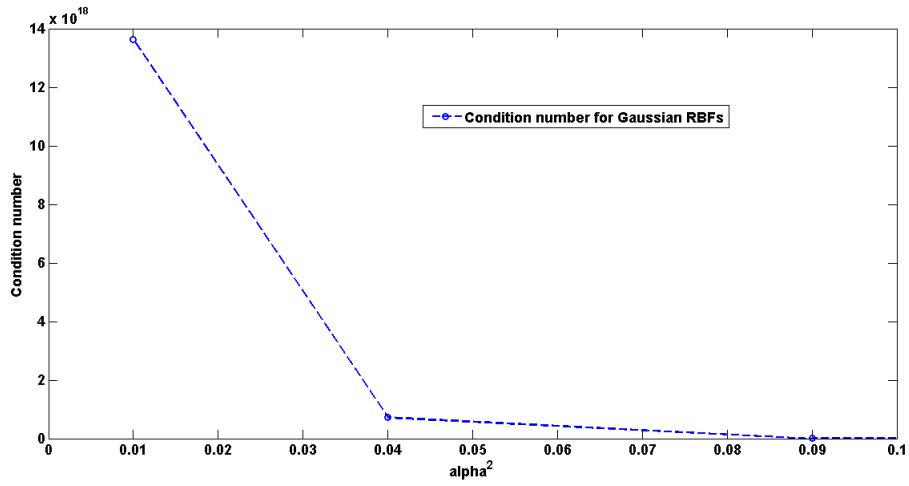


Figure 3.12: Condition number of Gaussian RBFs for different values of alpha for $N = 200$.

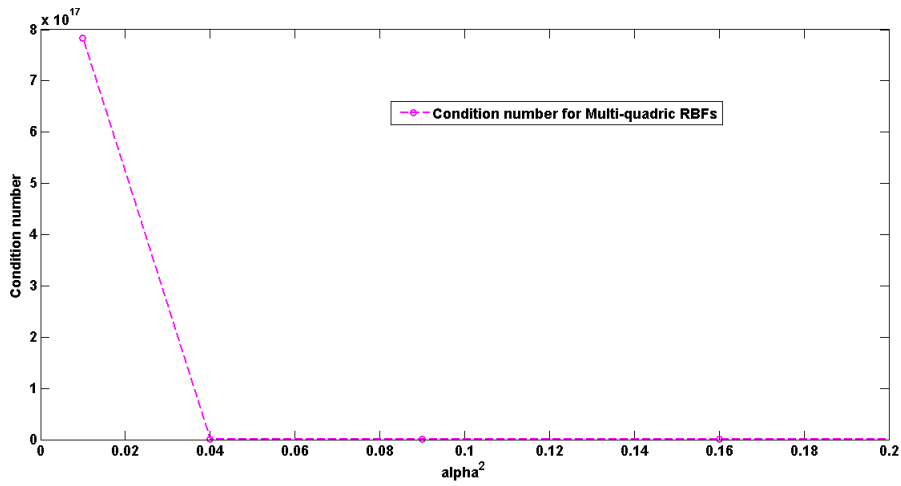


Figure 3.13: Condition number of MQ RBFs for different values of alpha for $N = 200$.

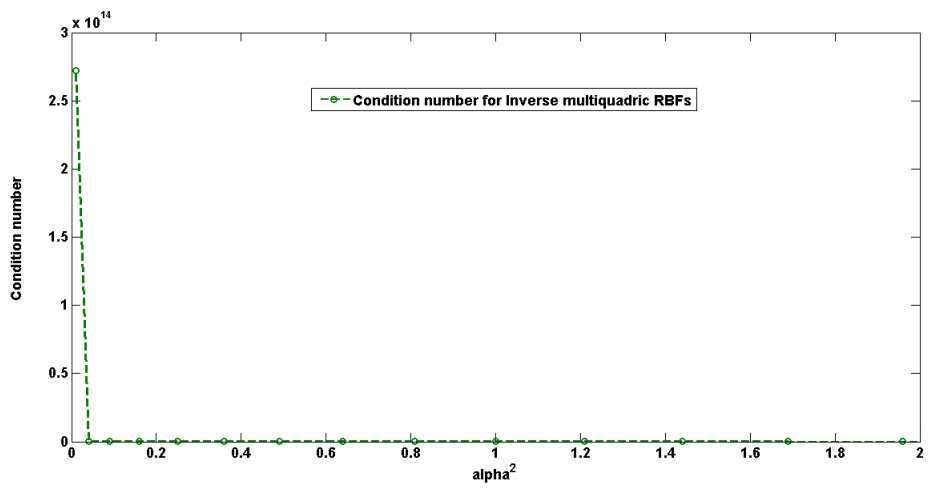


Figure 3.14: Condition number of IMQ RBFs for different values of alpha for $N = 200$.

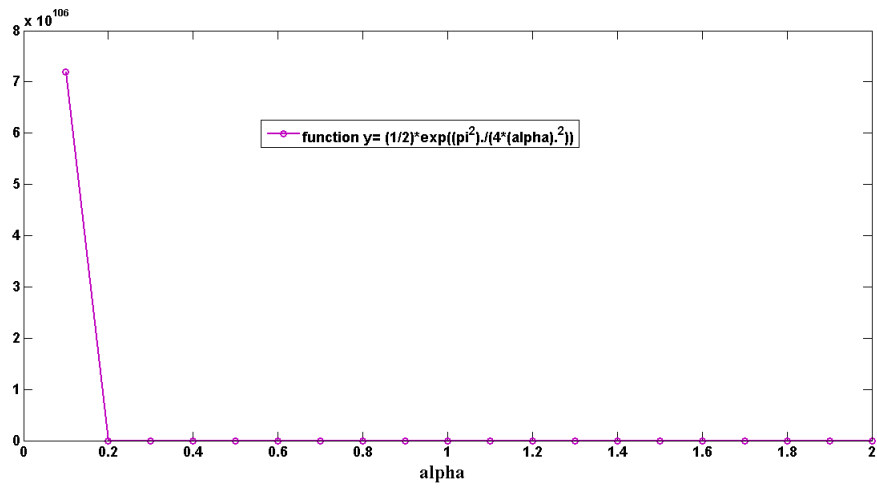


Figure 3.15: The graph of the functions $y = 1/2 \exp(\pi^2/4\alpha^2)$.

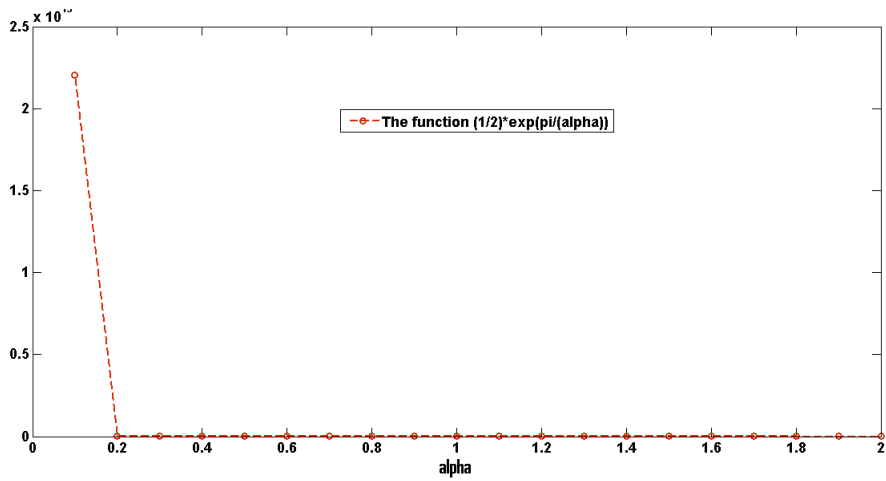


Figure 3.16: The graph of the functions $y = 1/2 \exp(\pi/\alpha)$.

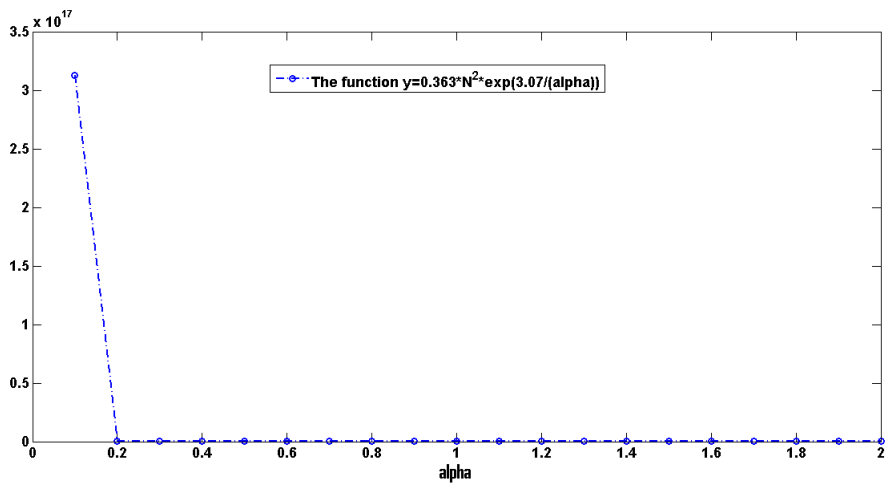


Figure 3.17: The graph of the functions $y = 0.363N^2 \exp(3.07/\alpha)$.

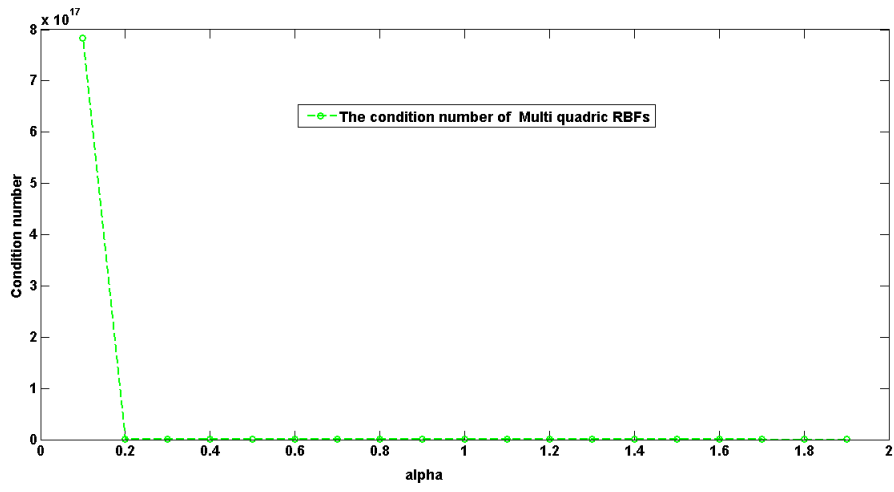


Figure 3.18: Condition number of MQ RBFs for different values of alpha for $N = 200$.

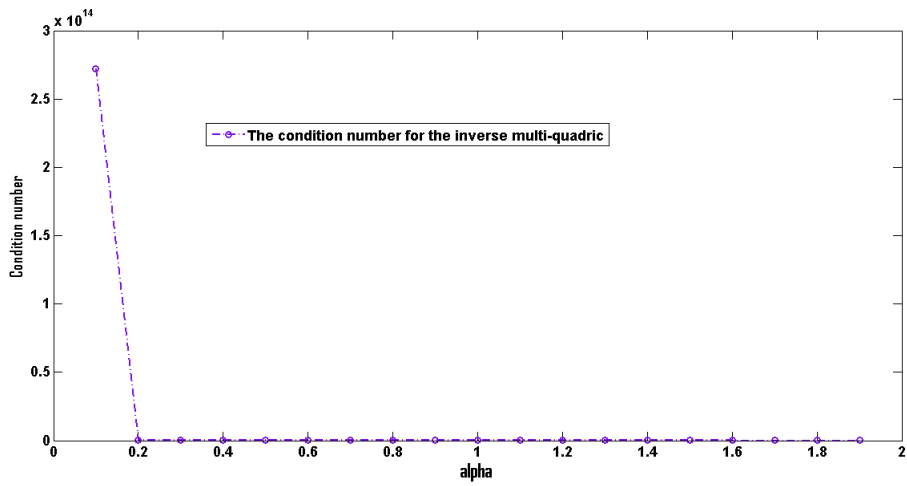


Figure 3.19: Condition number of IMQ RBFs for different values of alpha for $N = 200$.

Conclusion

Radial basis functions have proved very useful in computer graphics and neural networks and are growing in popularity for solving partial differential equations. A small shape parameter and a small fill distance are both desirable for accuracy, but both cause ill conditioned problems. The accuracy of RBFs meshless greatly depends on the user defined radial basis centers and the shape parameter. The researchers are confirmed that even when circumventing the ill conditioning of the system matrix there usually is a value of the shape parameter which results in optimal approximation errors. So it is necessary to find a strategy between the good accuracy and the well posed interpolation problem and therefore looks for a good balance between accuracy and stability.

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Abstract

Radial basis functions have proved very useful in computer graphics and neural networks and are growing in popularity for solving partial differential equations. It is known that the RBF matrix interpolation is very ill-conditioned. This is very unfortunate because it is known that RBF accuracy generally increases in the "flat" limit and is unreservedly awful in the opposite limit of RBFs. The subject of this dissertation is to review some essential preliminaries on the scattered data interpolation by RBFs. We also present a numerical method to solve nonlinear Fredholm Volterra integral equations. The method is based on the approximation of the solutions of these equations by using RBFs. For this aim, we take the Gaussian, Multiquadric and inverse multiquadric RBFs to approximate the solution. One of the subjects is to see the effect of the shape parameter on the condition number of matrix interpolation for some species of radial basis functions (RBFs), mostly on uniform grids.

Key-Words : Radial basis function, shape parameter, Volterra Fredholm integral equation, condition number, interpolation.

Résumé

Les fonctions de base radiales ont montrées leurs utilisations dans le domaine de l'infographie et des réseaux neuronaux et il sont très populaire pour la résolution des équations aux dérivées partielles. Il est connu que la matrice d'interpolation par RBF est très mal conditionnée. Ceci est très regrettable car il est connu que la précision des RBFs augmente généralement dans la limite "plate" et est sans réserve dans la limite opposée des RBFs. L'objectif de ce mémoire est de revoir quelques préliminaires essentiels sur l'interpolation de données dispersées par les RBFs. On présentons aussi une méthode numérique pour résoudre les équations intégrales non linéaires de Fredholm Volterra. La méthode est basée sur l'approximation des solutions de ces équations en utilisant des RBFs. Pour cet objectif, en prenant la gaussienne, multi-quadrique et multi-quadrique inverse pour approximer la solution. L'un des objectives est de voir l'effet du paramètre de base radial sur le conditionnement de la matrice d'interpolation pour certaines espèces de fonctions de base radiales (RBF), principalement sur des grilles uniformes.

Mots-Clés : Fonction de base radiale, paramètre de forme, équation intégrale de Volterra-Fredholm, nombre de conditions, interpolation.

ملخص

أثبتت وظائف الأساس الشعاعي أنها مفيدة جدًا في رسومات الكمبيوتر والشبكات العصبية وتتزايد شعبيتها في حل المعادلات التفاضلية الجزئية. من المعروف أن مصفوفة استقطاب الأساس الشعاعي شرطها سيء للغاية. من المعروف أن مصفوفة الاستقطاب باستعمال الأساس الشعاعي تقترب من أن تكون منفردة، لأنه من المعروف أن دقة الأساس الشعاعي تزداد عموماً باختيار أساس شعاعي واسع. موضوع هذه المذكرة هو مراجعة بعض الأساسيات حول استقطاب البيانات المبعثرة باستعمال الأساس الشعاعي، وتقديم طريقة عددية بهدف حل المعادلات التكاملية الغير خطية لفريدهولم فولتيرا. الفكرة الأساسية للطريقة تعتمد على تقريب الحلول المضبوطة لهذا النوع من المعادلات باستخدام الأساس الشعاعي. من أجل هذه الغاية استخدمنا أنواع مختلفة من الأساس الشعاعي منها الأساس المحوري والمعكوس له. والأساس الاسي. وإيضاً من بين الأهداف التي تمت مناقشتها رؤية مدى تأثير معامل الشكل على رقم الشرط لمصفوفة الأساس الشعاعي. في الأخير من خلال التجارب العددية المتنوعة نمتحن قيمة الشرط لمصفوفة الاستقطاب لبعض أنواع الأساس الشعاعي والتي تكون معظمها على شبكات موحدة.

الكلمات المفتاحية: دالة الأساس الشعاعي، إعدادات الشكل، معادلة فولتيرا فريدهولم المتكاملة، رقم الشرط، الاستقطاب.