Conditionality Analysis of the Radial Basis Function Matrix

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Abstract. The global Radial Basis Functions (RBFs) may lead to ill-conditioned system of linear equations. This contribution analyzes conditionality of the Gauss and the Thin Plate Spline (TPS) functions. Experiments made proved dependency between the shape parameter and number of RBF center points where the matrix is ill-conditioned. The dependency can be further described as an analytical function.

Keywords: Radial basis function · System of linear equations · Condition number · Matrix conditionality

1 Introduction

Interpolation and approximation of scattered data is a common problem in many engineering and research areas, e.g. Oliver et al. [1] use interpolation (kriging) method on geographical data, Kaymaz [2] finds usage of this technique in structural reliability problem. Sakata et al. [3] model wing structure with an approximation method, Joseph et al. [4] even create metamodels. The RBF methods are also used in the solution of partial differential equations (PDE) especially in connection with engineering problems.

To solve interpolation and approximation problems, we use two main approaches:

– Tesselated approach – it requires tesselation of the data domain (e.g. Delaunay triangulation) to generate associations between pairs of points in the tesselated cloud of points. Some algorithms were developed (Lee et al. [5] show two of them, Smolik et al. [6] show a fast parallel algorithm for triangulation of large datasets, Zeu et al. [7] recently use tesselation for seismic data etc.) for triangulation and tesselation. Even though it seems simple, tesselation is a slow process in general[1].

[1] The Delaunay triangulation has time complexity of $O\left(n^{\lceil d/2\rceil+1}\right)$, where d is number of tesselated dimensions.

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- Meshless approach – a method based on RBFs can be used, which does not require any from of tesselation. Hardy [8] shown that the complexity of this approach is nearly independent to the problem dimensionality, therefore it is a better alternative to tesselation in higher dimensions. On the other hand, RBF methods require solving a system of linear equations which leads to some problems as well.
  There are several meshless approaches e.g. Fasshauer [9] implements some of the meshless algorithms in MATLAB, Franke [10] compares some interpolation methods of the scattered data.
  Conditionality of the matrix of a linear system of equation is a key element to determine whether the system is well solvable or not.

RBF research was recently targeted:

- to find out RBF applicability for large geosciences data, see Majdisova [11],
- to interpolate and approximate vector data, see Smolik [12],
- to study robustness of the RBF data for large datasets, see Skala [13,14].
- to find out optimal variable shape parameters, see Skala [15].

This research is aimed to find optimal (or at least suboptimal) shape parameters of the RBF interpolation. This contribution describes briefly analysis of some of the most commonly used RBFs and determines its problematic shape parameters, causing ill-conditionality of the equation system matrix.

2 RBF Approximation and Interpolation

The basic idea behind the RBF approach is the partial unity approach, i.e. summing multiple weighted radial basis functions together to obtain complex interpolating function. The Fig. 1 presents two RBFs (marked by red color) forming an interpolating final function (blue one).

The RBF approach was introduced by Hardy [8] and modified in [16]. Since then, this method has been further developed and modified. Majdisova et al. [17] and Cervenka et al. [18] proposed multiple placement methods. There are also some behavioural studies of the shape parameters, e.g. searching the optimal ones from Wang et al. [19], Afiatdoust et al. [20] or using different local shape parameters from Cohen et al. [21], Sarra et al. [22], Skala et al. [15].

This contribution analyzes the worst cases of the RBF matrix conditionality in order to avoid bad shape parameters, therefore the bad shape parameters can be avoided.

2.1 RBF Method Principle

The RBF interpolation is defined by Eq. 1,

$$h(\mathbf{x}_i) = \sum_{j=1}^{N} \lambda_j \varphi(||\mathbf{x}_i - \mathbf{x}_j||) = \sum_{j=1}^{N} \lambda_j \varphi(r_{ij}) \tag{1}$$

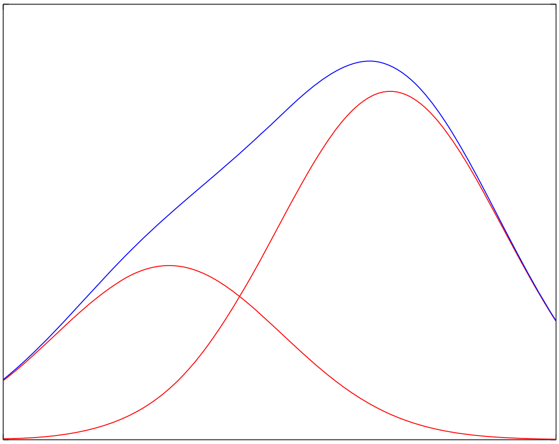

Fig. 1. Two RBFs (in red) and result of the addition (in blue). (Color figure online)

where $h(\mathbf{x}_i)$ is the resulting interpolant, N is the number of RBFs, $\lambda_\mathbf{i}$ is a weight of the i-th RBF, φ is the selected RBF and r_{ij} is a distance between points $\mathbf{x}_i$ and $\mathbf{x}_j$. The points $\mathbf{x}_j$ are all the points on the sampled original function, where the function value is known.

The RBF approximation is slightly different, see Eq. 2. The notation is the same as above, however, $\mathbf{x}_j$ are replaced by reference points $\xi_j, j = 1, \ldots, M$. Some arbitrary (sufficiently small $M \ll N$) number of points from the data domain are taken instead. More details can be found in Skala [23].

$$h(\mathbf{x}_i) = \sum_{j=1}^{M} \lambda_j \varphi(||\mathbf{x}_i - \xi_j||), \quad i = 1, \ldots, N \tag{2}$$

In both cases, i.e. approximation and interpolation, the equations can be expressed in a matrix form as:

$$\mathbf{A}\boldsymbol{\lambda} = \mathbf{b}, \quad \mathbf{b} = h(\mathbf{x}), \mathbf{A}_{ij} = \varphi_{ij} \tag{3}$$

In the interpolation case, the matrix $\mathbf{A}$ is a square matrix, while in the approximation case, the matrix $\mathbf{A}$ is rectangular and the result is an overdetermined system of linear equations. In this case, we do not obtain exact values for the already calculated reference points ξ_j.

2.2 RBF Classification

There are many RBFs and still new ones are being proposed e.g. Menandro [24]. In general, we can divide the RBFs into two main groups, "global" and "local" ones, see Fig. 3 and Fig. 2.

- **Global** RBFs influence the interpolated values globally. The matrix **A** will be dense and rather ill-conditioned. Typical examples of the global RBF are the Gaussian, the TPS or the inverse multiquadric RBFs.
- **Local** RBFs have limited influence to a limited space near its centre point (hypersphere, in general). The advantage of the local RBFs is that they lead to a sparse matrix **A**. RBFs belonging to this group are called "Compactly Supported" RBFs (CS-RBFs, in short).

Global RBFs are functions, which influence is not limited and its value may be nonzero for each value in its domain. The well-known ones are the Gaussian or the TPS functions. However, there are other functions, see e.g. Table 1 or Lin et al. [25]. Mentioned functions are illustrated in Fig. 2.

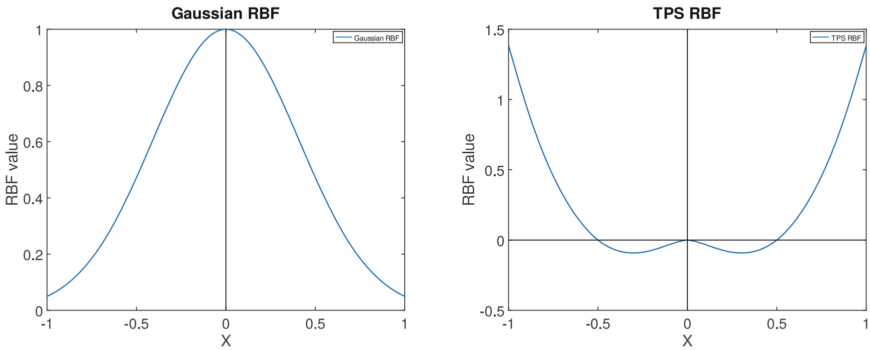

Fig. 2. Some of the global RBF functions.

Table 1. Various global RBF functions.

Name	Expression
Gaussian RBF	$e^{-\alpha r^2}$
TPS RBF	$\frac{1}{2} r^2 \log\left(\beta r^2\right)$
Multiquadratic RBF	$\frac{1}{1+(\epsilon r)^2}$
Inverse Multiquadratic RBF	$\frac{1}{\sqrt{1+(\epsilon r)^2}}$

The CS-RBF or compactly supported radial basis function is a function limited to a given interval. Some of CS-RBFs are presented on Fig. 3. Generally, these functions are limited to an interval (usually $r \in \langle 0, 1 \rangle$) otherwise the value equals zero. These functions are defined by Eq. 4, where $P(r)$ is a polynomial function, r is the distance of two points and q is a parameter.

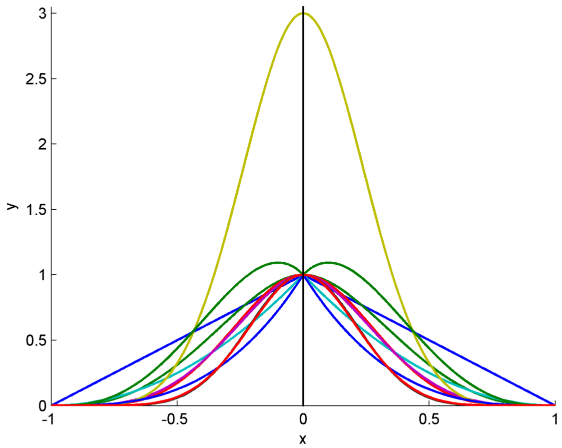

Fig. 3. Some of the CS-RBF functions. [26] (edited)

$$\varphi(r) = \begin{cases} (1-r)^q P(r) & 0 \leqslant r < 1, \\ 0 & r \geqslant 1 \end{cases} \tag{4}$$

It should be noted that some new CS-RBFs have been recently defined by Menandro [24].

3 Matrix Conditionality

Assuming a linear system of equations $\mathbf{Ax} = \mathbf{b}$, the condition number of the matrix $\mathbf{A}$ describes how the result (vector $\mathbf{b}$) can change when the input vector $\mathbf{x}$ is slightly modified. This number describes sensitivity to changes in the input vector. We aim for the lowest possible sensitivity, in order to get reasonable results. In terms of linear algebra, we can define conditionality of a normal matrix $\mathbf{A}$ using eigenvalues $\lambda_i \in \mathbb{C}^1$ as:

$$\kappa(\mathbf{A}) = \frac{|\lambda_{max}(\mathbf{A})|}{|\lambda_{min}(\mathbf{A})|} \tag{5}$$

where $\kappa(\mathbf{A})$ is the condition number of the normal matrix $\mathbf{A}$, $|\lambda_{max}(\mathbf{A})|$ is the highest absolute eigenvalue of the matrix $\mathbf{A}$ and $|\lambda_{min}(\mathbf{A})|$ is the lowest absolute eigenvalue of the matrix.

The higher the value $\kappa(\mathbf{A})$ is, the more sensitive the matrix $\mathbf{A}$ is, meaning that $\kappa(\mathbf{A}) = 1$ is the best option, forcing all eigenvalues λ to have the same value.

It is worth noting that the conditionality is closely related to the matrix determinant. In the case when the determinant is zero, we have at least one eigenvalue equaling zero, so the conditionality will be infinite, see Eq. 6.

$$\det(\mathbf{A}) = 0 \rightarrow |\lambda_{min}(\mathbf{A})| = 0 \rightarrow \kappa(\mathbf{A}) = +\infty \Leftrightarrow |\lambda_{max}(\mathbf{A})| \neq 0 \quad (6)$$

This is only a brief introduction to the matrix conditionality. Details can be found in e.g. Ikramov [27] or Skala [14], some experimental results can be found in Skala [28].

4 Experimental Results of RBF Approximation

In the RBF approximation problem, we normally have two main issues to deal with – selecting number of RBFs and its global shape parameter. To obtain a robust solution, the matrix $\mathbf{A}$ of the linear system of equations should not be ill-conditioned. We did some experiments to show how the condition number of the matrix $\mathbf{A}$ depends on the number of RBFs (N) used and a shape parameter (α or β, see below). To make things easier, all RBFs have been distributed uniformly on $x \in \langle 0, 1\rangle$ interval and have the same constant shape parameter.

4.1 Gaussian RBF

The Gaussian RBF is defined by Eq. 7. It is the unnormalized probability density function of a Gaussian distribution centred at zero and with a variance of $\frac{1}{2\alpha}$. Variable r denotes the distance from its centre points and α is the shape parameter.

$$\varphi(r, \alpha) = e^{-\alpha r^2} \quad (7)$$

Figure 4 presents dependence of matrix conditionality on Gaussian RBF shape parameter α and number of uniformly distributed RBF reference points.

A hyperbolic function (Eq. 8) was used to fit extremal points of each curve (Table 2).

Table 2. Analytical form of first 9 hyperboles.

Hyperbole	a	b	c	Hyperbole	a	b	c
1	7.64	38.36	−3.58	6	8.47	1387.35	−30.84
2	13.49	1.93	−7.98	7	17.98	1218.46	−49.14
3	9.17	277.29	−11.95	8	49.16	278.29	−78.53
4	9.44	509.55	−18.37	9	93.81	63.73	16.11
5	12.02	545.66	−31.8				

$$\beta = a + \frac{b}{N + c} \quad (8)$$

The plot at Fig. 5 describes the situation. These curves describe number of RBFs N and shape parameter α when the matrix is ill-conditioned.

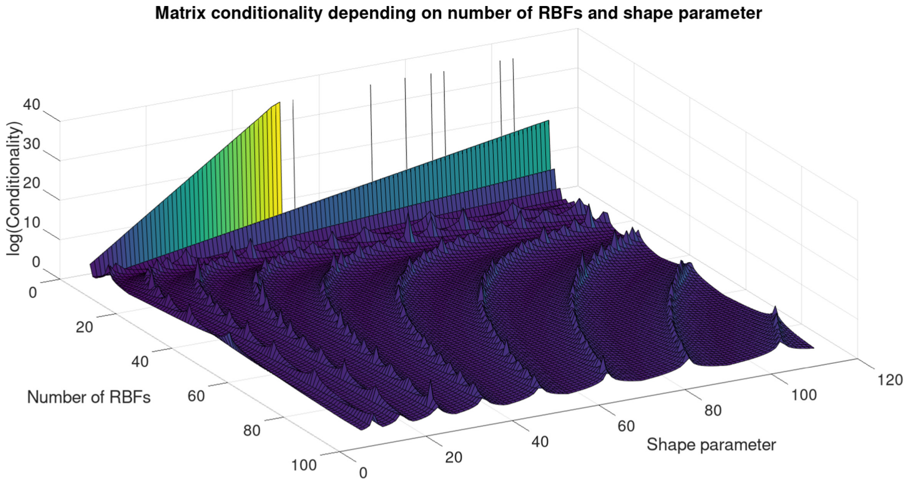

Fig. 4. Matrix conditionality values for Gaussian RBF.

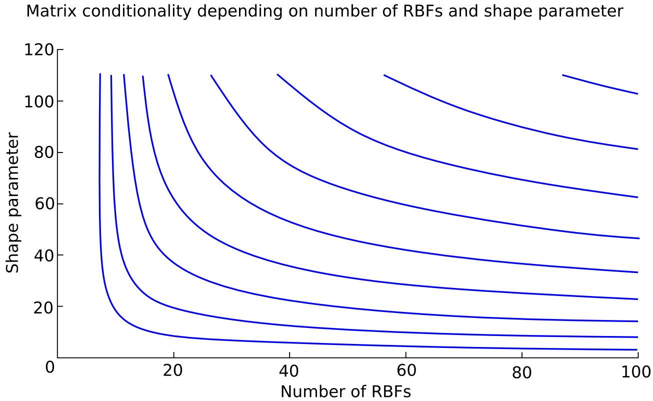

Fig. 5. Worst conditionality shape parameters α for Gauss RBF.

4.2 Thin Plate Spline RBF

The Thin Plate Spline (TPS) radial basis function is defined by the Eq. 9. The TPS was introduced by Duchon [29] and used for RBF approximation afterwards. Variable r is the same as in the Gaussian RBF – the distance from its centre point and parameter β is the shape parameter.

$$\varphi(r, \beta) = \frac{1}{2} r^2 \log\left(\beta r^2\right) \tag{9}$$

The Fig. 6 presents a result for a simulated experiment to the recent Gaussian RBF case using the TPS function instead. There is only one curve which has a hyperbolic shape similar to the Gaussian RBF case.

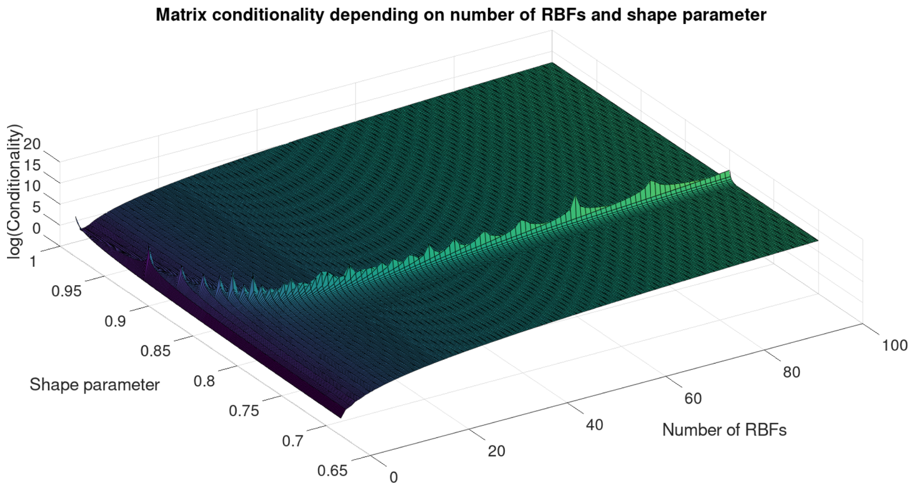

Fig. 6. Matrix conditionality values for TPS RBFs.

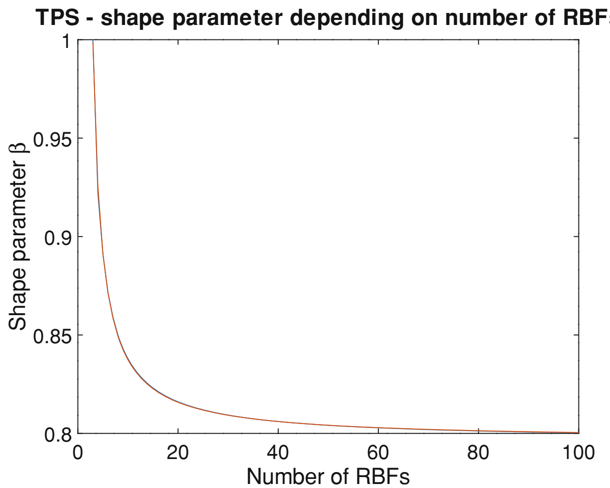

Fig. 7. Worst conditionality shape parameters β for the TPS RBF.

The Fig. 7 also represents the curve, when the matrix **A** is close to singular. The Table 3 presents dependency of the β_{exp} shape parameter for different N as an function when the matrix **A** is significantly ill-conditioned.

We obtained a hyperbolic function from the graph on Fig. 7 (coefficients are rounded to 2 decimal places).

$$\beta = 0.79 + \frac{0.36}{N - 1.24} \tag{10}$$

The Table 3 presents the shape parameters β_{calc} evaluated for small numbers of RBF functions according to Eq. 10.

The experimental results presented above led to a question, how the results are related from the analytical side. This led to the validation of experiments with two analytical results described in this section.

5 Theoretical Analysis

Let us calculate values of the TPS shape parameter β for $N = 3$ and $N = 4$ in a way that the matrix $\mathbf{A}$ will be ill-conditioned ($\kappa(\mathbf{A}) = +\infty$).

It should be noted that the multiplicative constant $\frac{1}{2}$ is ommited in the Eq. 11 as it has no influence to the conditionality evaluation. In the first case, i.e. $N = 3$, the RBF matrix $\mathbf{A}$ has the form (using equidistant distribution of RBF center points):

$$\mathbf{A}_3 = \begin{bmatrix} 0 & r^2 \log\left(\beta r^2\right) & (2r)^2 \log\left(\beta 4r^2\right) \\ r^2 \log\left(\beta r^2\right) & 0 & r^2 \log\left(\beta r^2\right) \\ (2r)^2 \log\left(\beta 4r^2\right) & r^2 \log\left(\beta r^2\right) & 0 \end{bmatrix} \tag{11}$$

Let us explore singularity of the matrix $\mathbf{A}_3$, when $\det(\mathbf{A}_3) = 0$, the determinant will have the form:

$$r^6 \begin{vmatrix} 0 & \log\left(\beta r^2\right) & 4\log\left(\beta 4r^2\right) \\ \log\left(\beta r^2\right) & 0 & \log\left(\beta r^2\right) \\ 4\log\left(\beta 4r^2\right) & \log\left(\beta r^2\right) & 0 \end{vmatrix} = 0 \tag{12}$$

As $r \neq 0$ for all pairs of different points, $\lim_{r\to 0} r^2 \log\left(r^2\right) = 0$ and equidistant point distribution.

For the sake of simplicity, we substitute $q = \log\left(\beta r^2\right)$, $a = \log 4$ and use formula $\log(ab) = \log a + \log b$ so we get:

$$\begin{gathered} \begin{vmatrix} 0 & q & 4(q+a) \\ q & 0 & q \\ 4(q+a) & q & 0 \end{vmatrix} = 0 \\ 8(q+a)q^2 = 0 \rightarrow q = 0 \vee q = -a \\ \log\left(\beta r^2\right) = -\log 4 = \log\frac{1}{4} \\ \beta r^2 = \frac{1}{4} \\ \beta = \frac{1}{4r^2} \end{gathered} \tag{13}$$

In the experiments, we used interval $x \in \langle 0, 1\rangle$ and with three points (0, 0.5, 1). The distance between two consecutive points r is 0.5, which led to $\beta = 1$. This exact value we obtained from experiments as well (see Table 3).

Table 3. β_{exp}-values for TPS RBF for some small N (number of RBFs) obtained by experiment as well as β_{calc} values calculated by Eq. 10

N	β_{exp}	β_{calc}	N	β_{exp}	β_{calc}	N	β_{exp}	β_{calc}
3	1.00000	0.99874	23	0.81338	0.81319	43	0.80535	0.80536
4	0.92206	0.92564	24	0.81264	0.81247	44	0.80515	0.80516
5	0.89118	0.89141	25	0.81197	0.81182	45	0.80496	0.80497
6	0.87182	0.87155	26	0.81135	0.81121	46	0.80477	0.80479
7	0.85909	0.85858	27	0.81078	0.81065	47	0.80459	0.80462
8	0.85002	0.84945	28	0.81025	0.81014	48	0.80442	0.80445
9	0.84324	0.84268	29	0.80976	0.80966	49	0.80426	0.80429
10	0.83799	0.83744	30	0.80930	0.80921	50	0.80410	0.80414
11	0.83379	0.83329	31	0.80888	0.80880	51	0.80395	0.80399
12	0.83037	0.82990	32	0.80848	0.80841	52	0.80380	0.80385
13	0.82753	0.82709	33	0.80811	0.80804	53	0.80366	0.80372
14	0.82512	0.82472	34	0.80776	0.80770	54	0.80353	0.80359
15	0.82306	0.82269	35	0.80743	0.80738	55	0.80340	0.80346
16	0.82128	0.82094	36	0.80711	0.80708	56	0.80328	0.80334
17	0.81973	0.81941	37	0.80682	0.80679	57	0.80316	0.80322
18	0.81835	0.81807	38	0.80654	0.80652	58	0.80304	0.80311
19	0.81713	0.81687	39	0.80628	0.80626	59	0.80293	0.80300
20	0.81605	0.81581	40	0.80603	0.80602	60	0.80282	0.80290
21	0.81507	0.81485	41	0.80579	0.80579	61	0.80272	0.80280
22	0.81418	0.81398	42	0.80557	0.80557	62	0.80262	0.80270

In the second case, i.e. $N = 4$, a similar approach has been taken. In this case the matrix $\mathbf{A}_4$ is defined as:

$$\mathbf{A}_4 = \begin{bmatrix} 0 & r^2\log\left(\beta r^2\right) & (2r)^2\log\left(\beta 4r^2\right) & (3r)^2\log\left(\beta 9r^2\right) \\ r^2\log\left(\beta r^2\right) & 0 & r^2\log\left(\beta r^2\right) & (2r)^2\log\left(\beta 4r^2\right) \\ (2r)^2\log\left(\beta 4r^2\right) & r^2\log\left(\beta r^2\right) & 0 & r^2\log\left(\beta r^2\right) \\ (3r)^2\log\left(\beta 9r^2\right) & (2r)^2\log\left(\beta 4r^2\right) & r^2\log\left(\beta r^2\right) & 0 \end{bmatrix} \tag{14}$$

Similarly as in the case for $N = 3$, we can write the $\det(\mathbf{A}_4)$ and declare the matrix singular if:

$$r^8 \begin{vmatrix} 0 & \log\left(\beta r^2\right) & 4\log\left(\beta 4r^2\right) & 9\log\left(\beta 9r^2\right) \\ \log\left(\beta r^2\right) & 0 & \log\left(\beta r^2\right) & 4\log\left(\beta 4r^2\right) \\ 4\log\left(\beta 4r^2\right) & \log\left(\beta r^2\right) & 0 & \log\left(\beta r^2\right) \\ 9\log\left(\beta 9r^2\right) & 4\log\left(\beta 4r^2\right) & \log\left(\beta r^2\right) & 0 \end{vmatrix} = 0 \tag{15}$$

Using the substitutions $q = \log\left(\beta r^2\right)$, $a = \log 4$ and $b = \log 9$, we obtain:

$$\begin{vmatrix} 0 & q & 4\left(q+a\right) & 9\left(q+b\right) \\ q & 0 & q & 4\left(q+a\right) \\ 4\left(q+a\right) & q & 0 & q \\ 9\left(q+b\right) & 4\left(q+a\right) & q & 0 \end{vmatrix} \tag{16}$$

This can be further expressed as:

$$\begin{aligned} &\left(4\left(q+a\right)\right)^4 + q^4 + q^2\left(9\left(q+b\right)\right)^2 \\ &= -2q^3\left(9\left(q+b\right)\right) - 2q\left(4\left(q+a\right)\right)^2\left(9\left(q+b\right)\right) - 2q^2\left(4\left(q+a\right)\right)^2 \\ &= 256(q+a)^4 + q^4 + 81q^2(q+b)^2 - 18q^3(q+b) \\ &- 288q(q+a)(q+b)^2 - 32q^2(q+a)^2 \end{aligned} \tag{17}$$

This leads to the cubic equation:

$$\begin{aligned} (383a - 144b)q^3 &+ (1216a^2 + 81b^2 - 576ab)q^2 \\ &+ (1024a^3 - 288a^2b)q + 256a^4 = 0 \end{aligned} \tag{18}$$

Solving this cubic equation (Eq. 18), one real and two complex (complex conjugate) roots are obtained:

$$\begin{aligned} q_1 &\approx -2.2784 \\ q_2 &\approx -1.1149 + 0.8239i \\ q_3 &\approx -1.1149 - 0.8239i \end{aligned} \tag{19}$$

As we have four points distributed uniformly on the interval $x \in \langle 0, 1\rangle$, the distance between two adjacent nodes is $r = \frac{1}{3}$. Now, using the real root of the Eq. 19, i.e. $q = -2.2784$, we can estimate the shape parameter β as follows:

$$\begin{aligned} q = \log\left(\beta r^2\right) &\approx -2.2784 \\ \beta r^2 &\approx e^{-2.2784} \approx 0.10245 \\ \beta &\approx \frac{e^{-2.2784}}{r^2} \\ \beta &\approx \frac{e^{-2.2784}}{\left(\frac{1}{3}\right)^2} = 9e^{-2.2784} \approx 0.92206 \end{aligned} \tag{20}$$

From the experiments, we obtained value $\hat{\beta} = 0.92206$ which is consistent with this theoretical estimation. Both these analytical examples support the argument that the experiments made are correct.

It should be noted, that if irregular point distribution is used, i.e. using Halton points distributions, the ill-conditionality get slightly worse.

6 Conclusion

In this paper, we discussed some properties of the two well-known RBFs. We find out that there are some regularities in the shape parameters, where the RBF matrix is ill-conditioned. Our experiments proved that there are no global optimal shape parameters from the RBF matrix conditionality point of view.

In the future, the RBF conditionality problem is to be explored for higher dimension, especially for $d = 2$, $d = 3$ and in the context of partial differential equations.

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