A Random Variable Shape Parameter Strategy for Radial Basis Function Approximation Methods

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Abstract

Several variable shape parameter methods have been successfully used in Radial Basis Function approximation methods. In many cases variable shape parameter strategies produced more accurate results than if a constant shape parameter had been used. We introduce a new random variable shape parameter strategy and give numerical results showing that the new random strategy often outperforms both existing variable shape and constant shape strategies.

Key words: Radial Basis Function, Multiquadric, Variable Shape Parameter

1. Introduction

Mathematicians have typically shied away from using a variable shape parameter strategy due to it adding an additional layer of complexity to the analysis of Radial Basis Function (RBF) methods. However Scientists and Engineers have shown in numerous works, including [2, 3, 8, 9, 5, 6, 7], that in terms of the accuracy of RBF methods that variable shape parameter strategies may have an advantage over a constant shape parameter strategy. In this work we introduce a new random variable shape parameter strategy.

First we briefly review RBF approximation methods for interpolation and steady PDEs. Then we describe some existing variable shape strategies as well

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as a new random variable shape strategy. Subsequently, the variable shape strategies are applied to a battery of test problems and then improvements to the random shape strategy are suggested for the case of widely scattered centers.

2. RBF Approximation

Given a set of ***centers*** $\mathbf{x}_1^c, \ldots, \mathbf{x}_N^c$ in $\mathbb{R}^d$, the RBF interpolant takes the form

$$s(\mathbf{x}) = \sum_{j=1}^{N} \alpha_j \phi(\left\| \mathbf{x} - \mathbf{x}_j^c \right\|_2, \varepsilon) \tag{1}$$

where

$$r = \| \mathbf{x} \|_2 = \sqrt{x_1^2 + \cdots + x_d^2}.$$

We focus on RBFs $\phi(r)$ that are infinitely differentiable and that contain a free parameter ε called the shape parameter. Some examples from this class of RBF are listed in table 1. In all the numerical examples, we have used the MQ which is representative of this class and is popular in applications. The coefficients α are chosen by enforcing the interpolation condition

$$s(\mathbf{x}_i) = f(\mathbf{x}_i) \tag{2}$$

at a set of nodes that typically coincide with the centers. Enforcing the interpolation conditions at N centers results in a $N \times N$ linear system

$$B\alpha = f \tag{3}$$

to be solved for MQ expansion coefficients α. The matrix B with entries

$$b_{ij} = \phi(\left\| \mathbf{x}_i^c - \mathbf{x}_j^c \right\|_2), \qquad i, j = 1, \ldots, N \tag{4}$$

is called the ***interpolation matrix*** or the ***system matrix*** and consists of the functions serving as the basis of the approximation space. For distinct center locations, the system matrix for the RBFs in table 1 is known to be nonsingular [10] if a constant shape parameter is used. To evaluate the interpolant at M points $\mathbf{x}_i$ using (1), the $M \times N$ ***evaluation matrix*** H is formed with entries

$$h_{ij} = \phi(\left\| \mathbf{x}_i - \mathbf{x}_j^c \right\|_2), \qquad i = 1, \ldots, M \text{ and } j = 1, \ldots, N. \tag{5}$$

Then the interpolant is evaluated at the M points by the matrix multiplication

$$f_{approx} = H\alpha. \tag{6}$$

Steady PDE problems are discretized by the RBF method in the following manner. If $\mathcal{L}$ is a linear differential operator, we have the linear boundary value problem

$$\mathcal{L}u = f \quad \text{ in } \Omega \tag{7}$$

where boundary conditions are imposed on all or parts of the boundary $\partial\Omega$ by a boundary operator $\mathcal{B}$ so that the PDE is well-posed. Let Ξ be a set of N distinct centers that are divided into two subsets. One subset contains N_I centers, $\mathbf{x}_I^c$, where the PDE is enforced and the other subset contains $N_{\mathcal{B}}$ centers, $\mathbf{x}_{\mathcal{B}}^c$, where boundary conditions are enforced. For simplicity, it is assumed that the centers are in an array that is ordered as $\Xi = [\mathbf{x}_I^c;\, \mathbf{x}_{\mathcal{B}}^c]$.

The RBF collocation method applies the operator $\mathcal{L}$ to the RBF interpolant (1) as

$$\mathcal{L}u(\mathbf{x}_i^c) = \sum_{j=1}^{N} \alpha_j \mathcal{L}\phi(\left\| \mathbf{x}_i^c - \mathbf{x}_j^c \right\|_2), \quad i = 1, \ldots, N_I \tag{8}$$

at the N_I interior centers and applies the operator $\mathcal{B}$ which enforces boundary conditions as

$$\mathcal{B}u(\mathbf{x}_i^c) = \sum_{j=1}^{N} \alpha_j \mathcal{B}\phi(\left\| \mathbf{x}_i^c - \mathbf{x}_j^c \right\|_2), \quad i = N_I + 1, \ldots, N \tag{9}$$

at the N_B boundary centers. In matrix notation, the right side of equations (8) and (9) can be written as $H\alpha$ where the evaluation matrix H that discretizes the PDE consists of the two blocks

$$H = \begin{bmatrix} \mathcal{L}\phi \\ \mathcal{B}\phi \end{bmatrix} \tag{10}$$

with the two blocks of H having elements

$$\begin{aligned} (\mathcal{L}\phi)_{ij} &= \mathcal{L}\phi(\left\| \mathbf{x}_i^c - \mathbf{x}_j^c \right\|_2), \qquad i = 1, \ldots, N_I, \quad j = 1, \ldots, N \\ (\mathcal{B}\phi)_{ij} &= \mathcal{B}\phi(\left\| \mathbf{x}_i^c - \mathbf{x}_j^c \right\|_2), \qquad i = N_I + 1, \ldots, N, \quad j = 1, \ldots, N. \end{aligned}$$

From the interpolation problem, we have that $\alpha = B^{-1}u$ where B is the system matrix with elements given by equation (4). The matrix that discretizes the PDE in space is the ***differentiation matrix***

$$D = HB^{-1}. \tag{11}$$

The differentiation matrix may discretize a single space derivative or an entire differential operator.

The steady problem (7) is discretized as

$$Du = f \tag{12}$$

and has solution

$$u = D^{-1}f = BH^{-1}f. \tag{13}$$

Even when employing a constant shape parameter, the evaluation matrix H can not be shown to always be invertible. In fact, examples have been constructed in which the evaluation matrix is singular [4]. Depending on the differential operator $\mathcal{L}$, the functions used to form the matrix H may not even be radial. Despite the lack of a firm theoretical underpinning, extensive computational evidence indicates that the matrix H is very rarely singular and the asymmetric method has become well-established for steady problems. If the boundary value problem is instead nonlinear, some type of iterative method will have to be used to evaluate the RBF approximation.

3. Variable Shape Strategies

Heuristically, it has been argued that using a variable shape parameter is a good idea. A variable shape parameter strategy refers to uses a possibly different value of the shape parameter at each center. This results in shape parameters that are the same in each column of the interpolation matrix or the evaluation matrix. One argument for using a variable shape parameter is that it leads to more distinct entries in the RBF matrices which in turn leads to lower condition numbers. A negative consequences of using a variable shape is that the system matrix is no longer symmetric. The standard results of the invertibility of the system [10] for a constant shape parameter no longer apply. However, some progress has been made to establish the invertibility of the system matrix when the shape is non-constant [1].

In [5], the formula

$$\varepsilon_j = \left[\varepsilon_{min}^2 \left(\frac{\varepsilon_{max}^2}{\varepsilon_{min}^2}\right)^{\frac{j-1}{N-1}}\right]^{\frac{1}{2}} \qquad j = 1, \ldots, N, \tag{14}$$

which gives a exponentially varying shape parameter, was suggested in order to have a different value shape parameter with each basis function in the expansion (1). Variable shape parameter strategy (14) was introduced for use as a formula for the shape parameter c in the original definition of the MQ, $\phi(r) = \sqrt{c^2 + r^2}$. The strategy works equally as well as formula for ε in the modern definition of the MQ in table 1. This is due to the reciprocal relationship between the shape definitions and the fact that it does not matter wether the shape parameter increases or decreases with the center number [5]. Further numerical experiments with the variable shape parameter strategy (14) can be found in reference [8]. In [8] it was shown that very accurate approximation results could be obtained if ε_{min}^2 and ε_{max}^2 varied by several order of magnitude. The strategy was successful even when the underlying function varied rapidly or had steep gradients. However, also in reference [8], it was shown that this recipe did not always work. One such example is on the surface of a sphere where a constant shape parameter worked the best.

Other possible variable shape parameter strategies include a linearly varying parameter

$$\varepsilon_j = \varepsilon_{min} + \left(\frac{\varepsilon_{max} - \varepsilon_{min}}{N-1}\right) j \qquad j = 0, 1, \ldots, N-1 \tag{15}$$

and the random shape strategy

$$\varepsilon_j = \varepsilon_{min} + (\varepsilon_{max} - \varepsilon_{min}) \times \text{ rand(1,N)} \tag{16}$$

that we are proposing in this work. The function rand is the Matlab function that returns N uniformly distributed pseudo-random numbers on the unit interval. Equation (16) returns N random shape parameters between ε_{min} and ε_{max}, and unlike the strategies (14) and (15), the shape parameters are not monotone increasing or decreasing. From our experience, the exponential (14) and linearly (15) varying shape parameters have a tendency to result in approximations that have larger errors in regions where the shape parameter, ε, is largest. Due to its non-monotone nature, the proposed random variable shape parameter strategy (16) seems to alleviate this problem while at the same time providing a variable shape that improves the conditioning of the resulting matrices.

In figure 1, the shape parameter values from the various selection strategies are illustrated with $N = 40$ centers and $\varepsilon_{max} = 10$ and $\varepsilon_{min} = 1$.

4. Numerical Examples

In all plots, the random variable shaped parameter results are marked with a solid line, exponential with a dotted line, constant with a dashed line, and linear with a dashed dotted line. All error plots display the maximum error.

4.1. 1d interpolation

Our first numerical experiment involves interpolating four 1d functions with different properties. The functions are an exponential and trigonometric combination

$$f_1(x) = \exp(x^3) + \cos(2x),$$

a second degree polynomial

$$f_2(x) = x^2 + 2x + 1,$$

a function with a steep front in the center of the domain

$$f_3(x) = \arctan 5x,$$

and a constant function

$$f_4(x) = 1.$$

The results are compared over a range of the average shape parameter

$$\varepsilon_{avg} = \frac{1}{2}(\varepsilon_{max} + \varepsilon_{min}).$$

The distance $K = \varepsilon_{max} - \varepsilon_{min}$ has been specified as $K = 1$ in all reported results. The numerical experiments were run over a wide range of K values and taking $K \approx 1$ typically resulted in the best accuracy. Taking $K \gg 1$ severely degraded the accuracy when compared to using small K.

In figure 2 the accuracy results are shown from the four shape parameter strategies being applied to the four functions above. In the left column of the figure $N = 60$ equally spaced centers have been used and the interpolant was evaluated at $M = 200$ equally spaced evaluation points. In the right column $N = 180$ equally spaced centers have been used and the interpolant was evaluated at $M = 300$ equally spaced evaluation points. The condition numbers of the system matrix versus the average shape parameter is shown in figure 3. The condition numbers of the system matrices are very similar for all four shape strategies with both $N = 60$ and $N = 180$. With $N = 60$, the variable random shape strategy produces the best accuracy by several decimal places for functions f_1, f_2, and f_4 and accuracy comparable to the other three strategies for function f_3. Function f_3 is revisited in section 5 where the variable random shape strategy is modified to effectively handle widely scattered center locations. With $N = 180$ the variable random shape strategy again results in the best accuracy. This results are very accurate even though the condition number of the system matrices (right image of figure 3) are extremely large.

4.2. 2d interpolation

As a two dimensional example, the function

$$f(x, y) = e^{xy} \tag{17}$$

is interpolated on a domain that is the portion of the circle centered at the origin with radius $\sqrt{2}$ that is in the first quadrant with $x \geq 0$ and $y \geq 0$.

In a large number of numerical experiments, the variable random shape strategy consistently produced more accurate results using equally spaced centers than the three other strategies that have been considered. When the centers become scattered, the variable random shape strategy seems to loose its advantage over the other two variable shape strategies. With scattered centers, all three variable shape strategies produce approximately the same accuracy which is considerably better than if a constant shape had been used. In section 5, the variable random shape strategy will be modified to perform better on scattered centers.

Using the $N = 1297$ uniformly spaced centers in the top left image of figure 4 to interpolate function (17) results in the accuracy versus the average shape parameter shown in the left image of figure 5. The variable random shape strategy is about two decimal places more accurate over a large range of average shape parameters than are the other three strategies. If instead the $N = 1297$ scattered centers in the bottom left image of figure 4 are used, then the three variable shape strategies produce about the same accuracy which is in some cases about four decimal places more accurate than when using a constant shape.

4.3. 2d linear BVP

We use the two dimensional linear Elliptic boundary problem

$$\begin{aligned} u_{xx} + u_{yy} &= f(x,y), \qquad (x,y) \in \Omega \\ u(x,y) &= g(x,y), \qquad (x,y) \in \partial\Omega \end{aligned} \tag{18}$$

as a steady PDE test problem for the shape parameter strategies. The domain Ω is taken to be a circle of radius $1/2$ that is centered at the origin. The $N = 250$ centers that are used in the example are shown in figure 6.

First we specify f and g in (18) so that the exact solution is the exponential function

$$u(x,y) = e^{(x+2y)}. \tag{19}$$

Next f and g are specified in (18) so that the exact solution is the relatively flat function

$$u(x,y) = \frac{65}{65 + (x-0.2)^2 + (y+0.1)^2}. \tag{20}$$

The accuracy versus a range of average shape parameters is shown in figure 7. In both problems the constant shape parameter is the least accurate. Of the three variable shape strategies, the random strategy is slightly more accurate on both problems.

5. Improved Random Variable Shape for Scattered Data

Function $f_3(x)$ is flat near the boundaries but has a steep gradient near $x = 0$ as shown in left image of figure 8. Thus the uniform placement of center used for this function in section 4.1 is not the best choice. A better choice would be a distribution of centers that clusters more densely around $x = 0$ as is specified by equation

$$x_j = \frac{2}{\pi} \arcsin\left(\frac{-1+2j}{N-1}\right), \quad j = 0, \ldots, N-1 \tag{21}$$

and is illustrated in the right image of figure 8. On such nonuniform grids, the random variable shape parameter was the least accurate of the four methods tested. To improve the performance of the random variable shape parameter with scattered centers, information about the minimum distance of a center to its nearest neighbor h_n can be incorporated into the algorithm as

$$\varepsilon_j = \frac{\mu}{h_n} \left[\varepsilon_{min} + (\varepsilon_{max} - \varepsilon_{min}) \times \text{ rand(1,N) } \right] \tag{22}$$

where $\mu > 0$ is a user specified parameter.

Using the $N = 60$ centers in the right image of figure 8 and setting $\mu = 1/20$ we get the shape parameters shown in figure 10. The accuracy of the modified random variable shape strategy is compared to the accuracy of the other three strategies in the left image of figure 9. The modified random variable shape strategy is considerably more accurate over the entire range of average shape parameters. Additionally, the condition number of the system matrix of the modified random method is considerably smaller over most of the average shape range in comparison to the other three methods.

Note that while the information about the minimum distance of a center to its nearest neighbor could be incorporated into the variable linear and exponential shape strategies as well, but then they would produce shapes that would not be linear or exponentially varying.

6. Conclusions

We have compared four shape parameter strategies and applied them to a battery of test problems. One strategy uses a constant shape while the other three use a different value of the shape parameter at each center. The use of a constant shape produced the least accurate result on the test problems. In interpolation problems, a new random variable shape parameter strategy produced the most accurate results if the centers were uniformly spaced. If the random variable shape parameter is modified to incorporate information about the minimum distance of a center to its nearest neighbor the random shape strategy again produced the most accurate results, even with very irregularly spaced centers. On two Poisson problems, the constant shape was again the least accurate. The random variable strategy resulted in slightly better accuracy on the steady PDE problems than when using the variable linear and exponential shapes. A small distance between ε_{min} and ε_{max}, such as $K = 1$, led to the most accurate results in all three variable shape strategies.

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Name of RBF	Definition
Multiquadric (MQ)	$\phi(r,\epsilon) = \sqrt{1+\epsilon^2 r^2}$
Inverse Multiquadric (IMQ)	$\phi(r,\epsilon) = 1/\sqrt{1+\epsilon^2 r^2}$
Inverse Quadratic (IQ)	$\phi(r,\epsilon) = 1/(1+\epsilon^2 r^2)$
Gaussian (GA)	$\phi(r,\epsilon) = e^{-\epsilon^2 r^2}$

Table 1: Global, infinitely smooth RBFs containing a shape parameter.

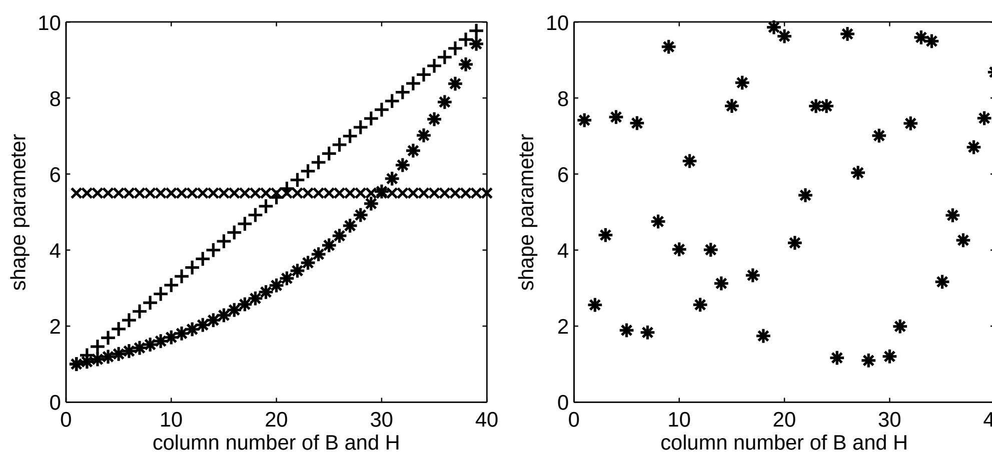

Figure 1: Left: constant, linearly varying, and exponentially varying, shape parameters. Right: random shape parameters.

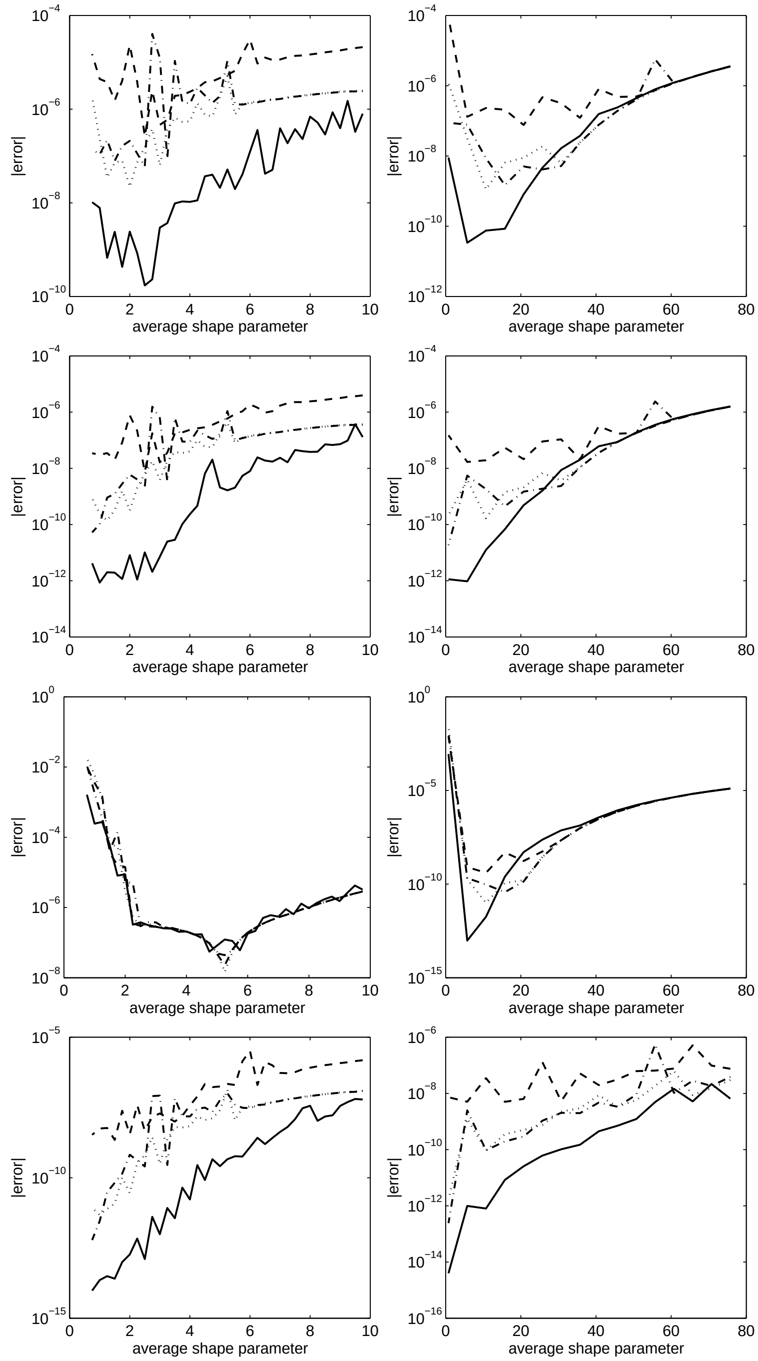

Figure 2: Accuracy over a range of average shape parameters. Row 1 function f_1, row 2 function f_2, row 3 function f_3, and row 4 function f_4. Left: $N = 60$. Right: $N = 180$.

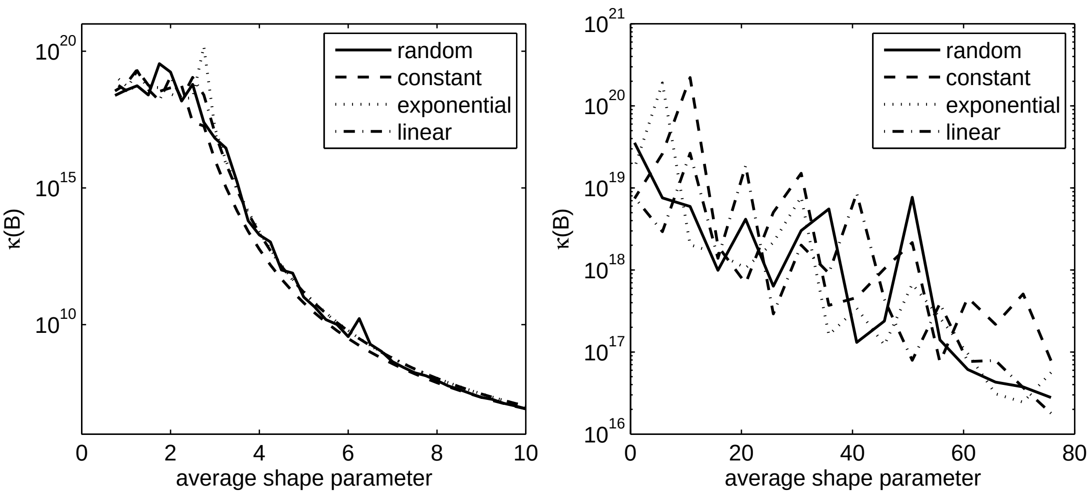

Figure 3: Condition number of the system matrix versus the average shape parameter. Left: $N = 60$. Right: $N = 180$.

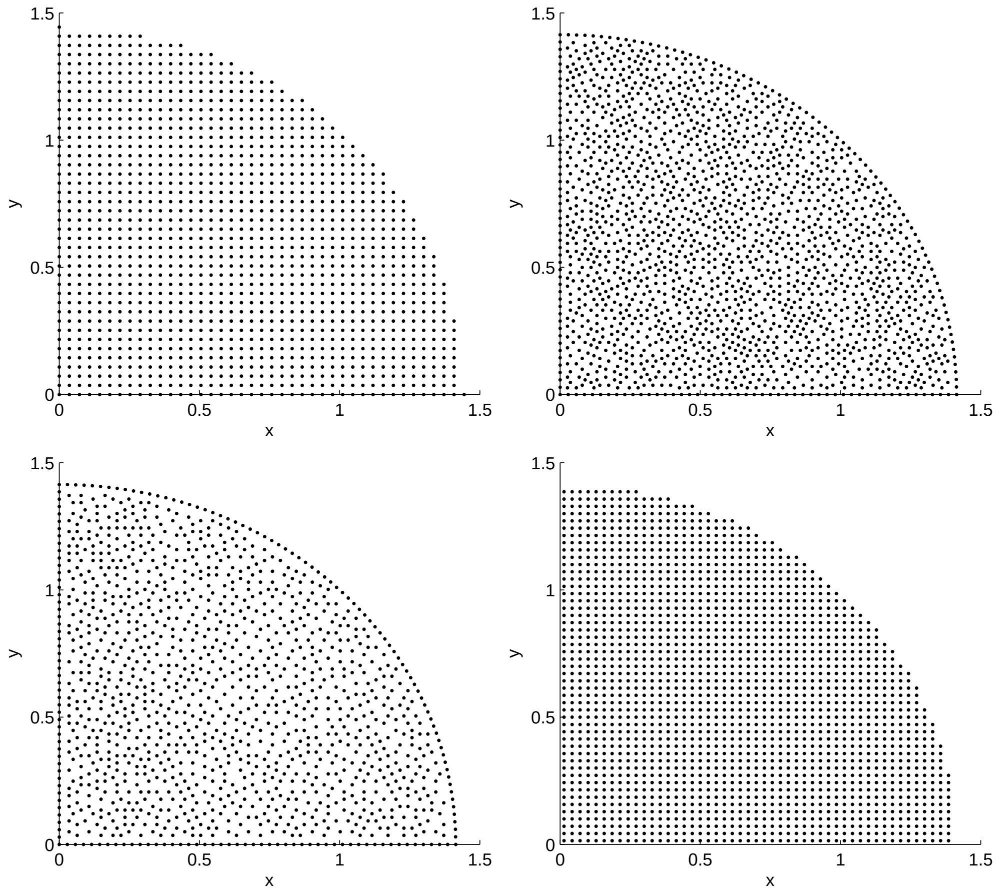

Figure 4: Centers and evaluation points for interpolating function (17). Top left: $N = 1297$ uniformly spaced centers. Top right: $M = 1917$ scattered evaluation points. Bottom left: $N = 1297$ scattered centers. Bottom right: $M = 1917$ uniformly spaced evaluation points.

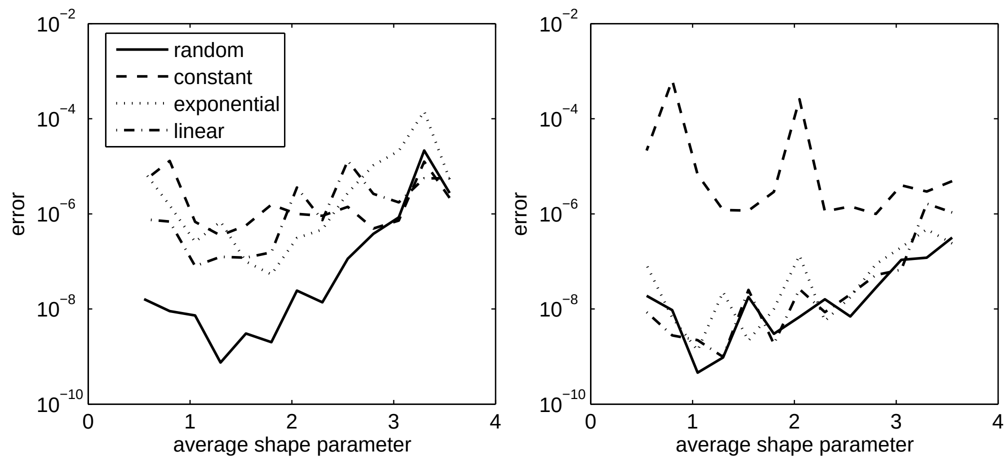

Figure 5: Accuracy in interpolation function (17) over a range of average shape parameters. Left: Using $N = 1297$ uniformly spaced centers shown in the top left image of figure 4. Right: Using $N = 1297$ scattered centers shown in the bottom left image of figure 4

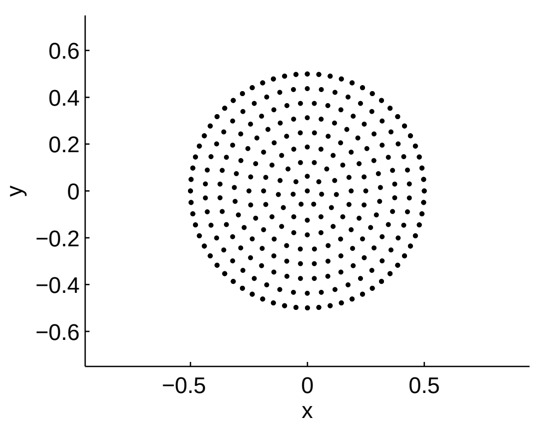

Figure 6: Centers for the Poisson problem (18).

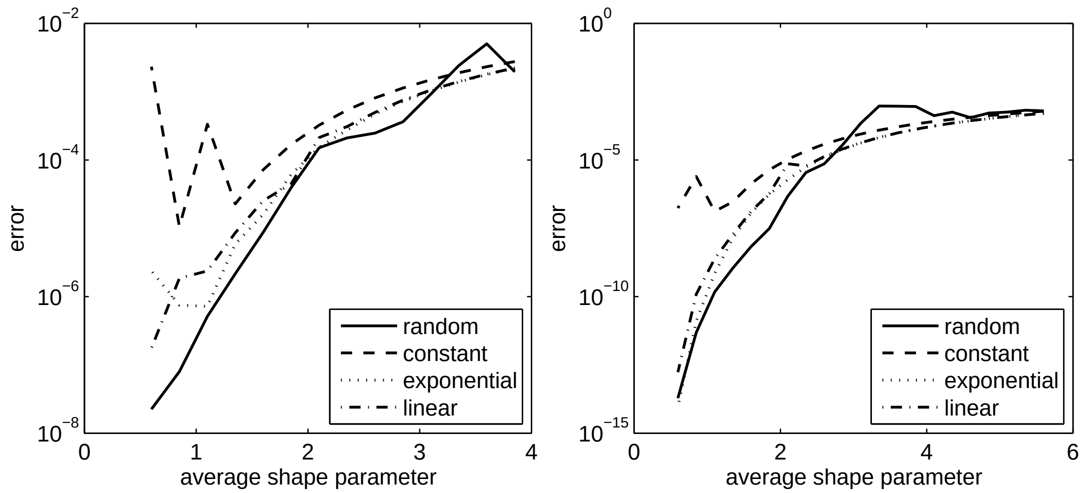

Figure 7: Accuracy versus average shape parameter. Left: Poisson problem with solution (19). Right: Poisson problem with solution (20).

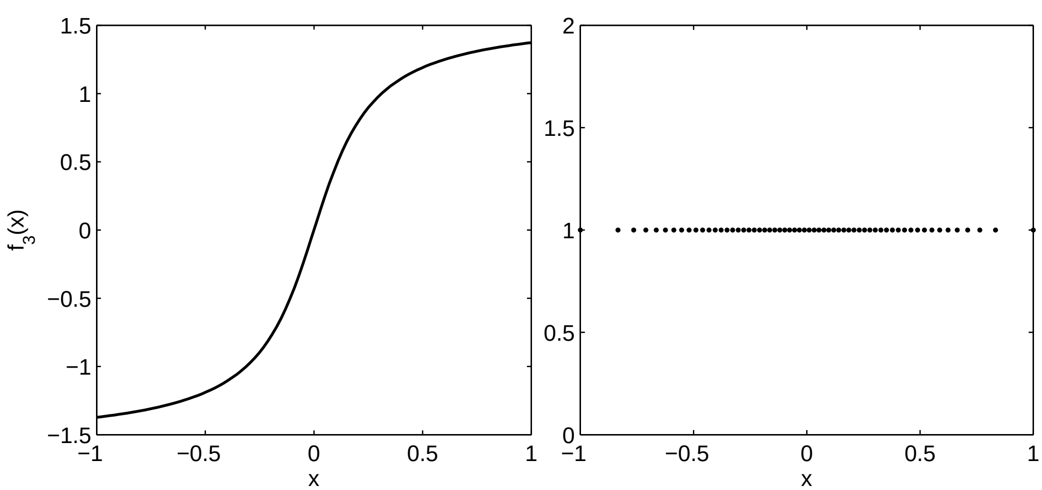

Figure 8: Left: $f_3(x)$. Right: 60 centers located according to equation (21).

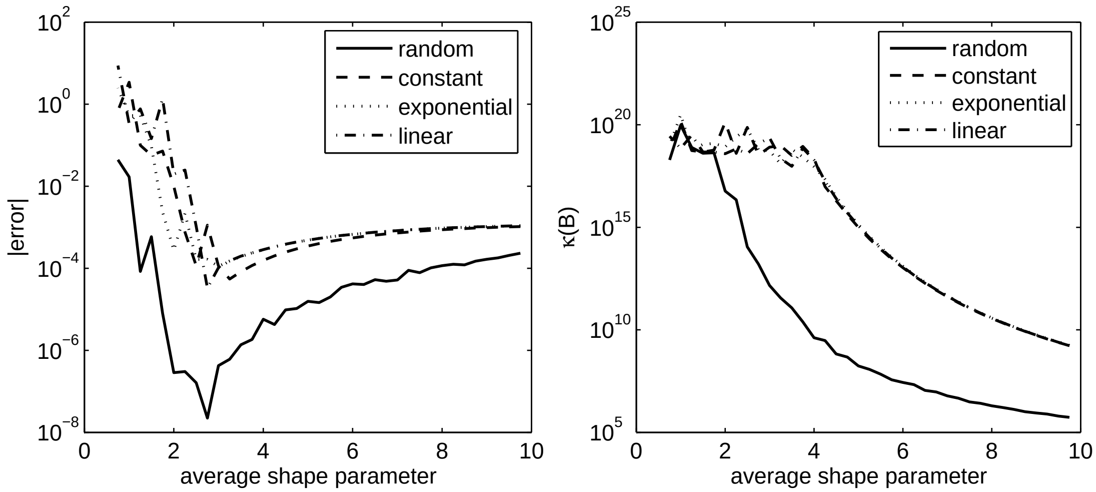

Figure 9: Left: Accuracy versus average shape parameter. Right: System matrix condition numbers versus average shape parameter.

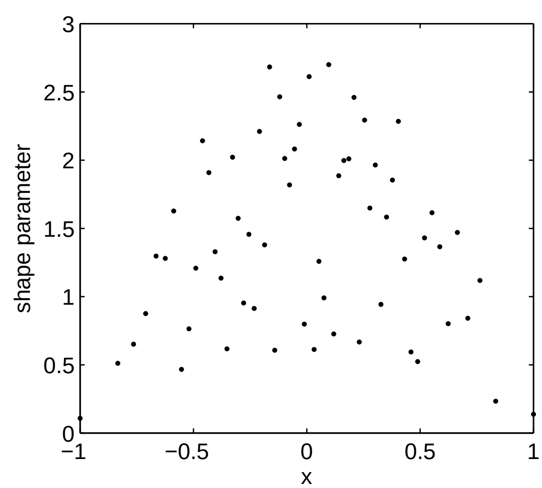

Figure 10: Variable random shape parameters with minimum separation distance incorporated.