An Investigation of Choosing Shape Parameter in the Radial Basis Function Approximation

By

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Thesis submitted to the University of Sri Jayewardenepura for the award of the Degree of Master of Science/Diploma in Industrial Mathematics

DECLARATION

The work described in this thesis was carried out by me under the supervision of Dr.P.A. Jayantha and a report on this have not been submitted in whole or in part to any university or any other institution for another Degree/Diploma.

To be the best of my knowledge the above particulars are correct.

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DECLARATION

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Degree: M.Sc in Industrial Mathematics

Examining Committee:

I/We certify that the above statement made by the candidate is true and that this thesis is suitable for submission to the University for the purpose of evaluation.

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f1 : $y = (x-.5)^2$, $x \in [-1.0, 1.0]$ f2 : $y = (1+\sin 6x)/2$, $x \in [-1.0, 1.0]$ f3 : $y = e^{5x}$, $x \in [-1.0, 1.0]$ f4 : $y = \tanh(4x)$, $x \in [-1.0, 1.0]$	f5 : $y = \log(x+2.5)$, $x \in [-1.0, 1.0]$ f6 : $y = \frac{1}{(1+(x-.25)^2)}$, $x \in [-1.0, 1.0]$ f7 : $y = .35(x+2.5)^{0.7}$, $x \in [-1.0, 1.0]$ f8 : $y = 3\tan^{-1}(2x)$, $x \in [-1.0, 1.0]$

Plots of these functions can be found in Appendix B(see Figures 1.1-1.8).The following data sets are taken from Tarwater[7] for numerical simulations.

9 unequally spaced points

$S_1 = \{-1.0, -.95, -.9, -.8, -.7, -.1, .5, .75, 1.0\}$

9 Chebyshev points

$S_2 = \{-.985, -.866, -.643, -.342, 0, .342, .643, .866, .985\}$

17 unequally spaced points

$S_3 = \{-1.0, -.975, -.95, -.925, -.9, -.85, -.8, -.75, -.7, -.4, -.1, .2, .5, .625, .75, .875, 1.0\}$

17 Chebyshev points

$S_4 = \{-.996, -.962, -.895, -.798, -.674, -.526, -.361, -.184, 0, .184, .361, .526, .674, .798, .895, .962, .996\}$

25 unequally spaced points

$$S_5 = \begin{Bmatrix} -1.0, -.975, -.95, -.925, -.9, -.875, -.85, -.825, -.8, -.75, -.725, -.7, -.55, -.4, -.25, -.1, 05, .2, .35, \\ .5, .625, .7, .75, .875, 1.0 \end{Bmatrix}$$

25 Chebyshev points

$$S_6 = \begin{Bmatrix} -.998, -.982, -.951, -.905, -.844, -.771, -.685, -.588, -.482, -.368, -.249, -.125, 0, .125, .249, \\ .368, .482, .588, .685, .771, .844, .905, .951, .982, .998 \end{Bmatrix}$$

Altogether 8 test functions are interpolated over 6 data sets. One-dimensional MQ, RMQ and GA radial basis functions were used to interpolate various data generated by 8 functions. RMSE is used as a measure of 'good fit'. The lower the RMSE, the better the fit. This RMSE is computed over a uniform mesh containing 50 points.

'Optimal c^2 'is the value which corresponds to the lowest RMSE. But finding the optimal c^2 is an open research question. So far no analytical techniques have been developed to find this value. In our numerical experiments plots were made of log(c^2) versus log(RMSE). By looking at these curves we can conclude such a value does exist. So when we refer as 'optimal c^2' in this document what we mean is an approximate value of this elusive value.

Many researchers have proposed various schemes to find the optimal c^2. The pioneers of RBF approximation techniques believed the optimal c^2 is solely dependent only on the data sets interpolated. Hardy [1] who first used RBF approximation techniques and Foley [8] suggested a scheme depending on the average distance between data points.

Foley [8] simplified the calculation using $\frac{(x_{\max} - x_{\min})^2}{N}$ as an approximation of the average distance squared from a data point (x_i, y_i). Franke [9] proposed schemes taking into account the 'scattering' of the dataset the function interpolated. Tarwater [7] made some modifications to Franke's scheme incorporating the average distance between points as a factor.

The followings are the analyzed schemes:

1) Hardy's scheme

$$c^2 = 0.815^2 d^2, \text{ where } d = \frac{\sum d_i}{N},\ d_i = \min_{i \neq j} |x_i - x_j|$$

2) Franke's scheme

$$c^2 = \frac{1.25^2 (x_{\max} - x_{\min})^2}{N}$$

3) Foley's method

$$c^2 = 4\frac{(x_{\max} - x_{\min})^2}{N^2}$$

4) Modified Franke's method 1

$$c^2 = 1.25^2 (x_{\max} - x_{\min}) \max DBP$$

5) Modified Franke's method 2

$$c^2 = 1.25^2 \frac{(x_{\max} - x_{\min})^2}{N} \frac{\max DBP}{\min DBP}$$ where $\max DBP = \max(|x_i - x_j|, |i - j| = 1)$ and

$\min DBP = \min(|x_i - x_j|, |i - j| = 1)$.

In our numerical experiments for a test function, a dataset and given radial basis function log(RMS error) is plotted against log(shape parameter c^2) at first. 20 evaluations were used to plot this curve. (see Apendix code A 1.1.3)

In shape parameter c^2 table optimal c^2 column is divided into two columns namely optimal1 c^2, optimal2 c^2 (see Table 2.1.1). Optimal1 c^2 is the value of c^2 which gives the minimum RMSE. This value is obtained using log(c^2) versus log(RMSE).

As the consequence of this we were able to get some idea about the range we have to look for the 'optimal c^2'. Then we have to 'fine-tune' this range to obtain a c^2 not only with lowest RMSE but also it must be computationally stable. Optimal 2 c^2 is the value obtained as mentioned above. 20 evaluations are used to plot this curve and shape parameter c^2 vs. RMSE is plotted (see Apendix code A 1.1.4).

For instance when function f2 was interpolated over dataset S1 using MQ, we were able determine optimal 1 c^2 as 10(see Table 2.1.1). When fine-tuning this value, we get a local minimum at 6.15 and as consequence optimal 2 c^2 (see Figure 2.1.1, 2.1.2). But for some cases we were unable to reach a local minimum. In those cases we have to opt for stable computation. When fine-tuning c^2 we have to increase c^2 till the graph remains smooth. Beyond this point the curve becomes 'jagged' indicating instability in computation. In these cases the 'breakdown' point is the optimal2 c^2 value.

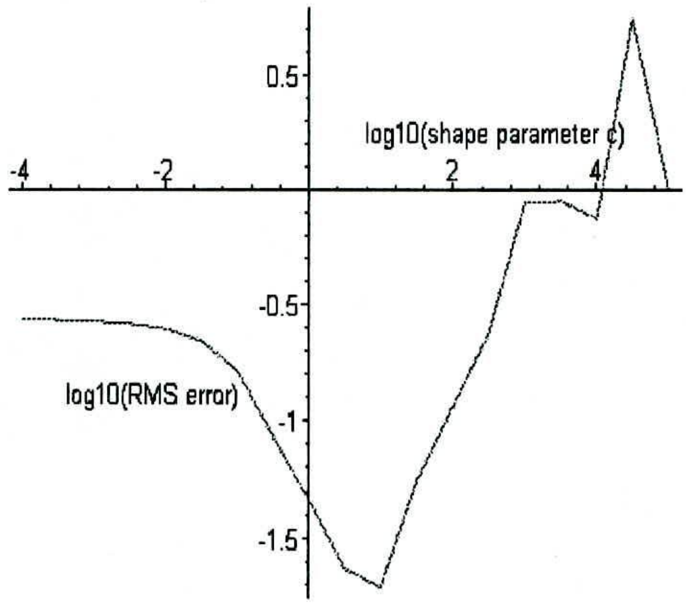

Figure 2.1.1 log (shape parameter c) vs. log (RMSE) of function f2 interpolated over dataset S1 using MQ RBF.

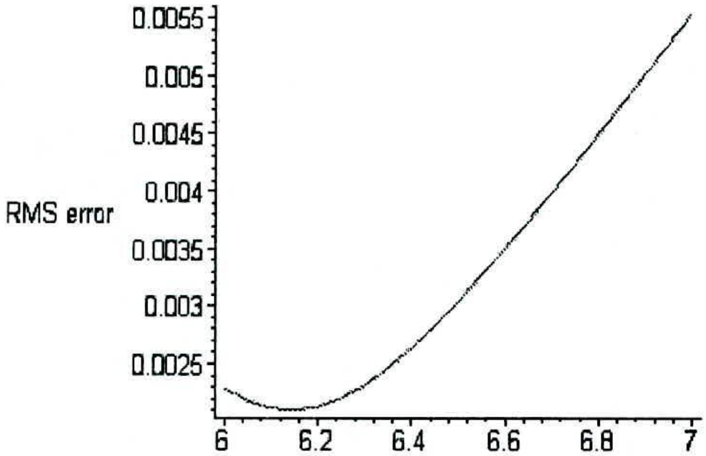

Figure 2.1.2. Shape parameter *c* vs. RMSE of function f2 interpolated over dataset S1 using MQ RBF.

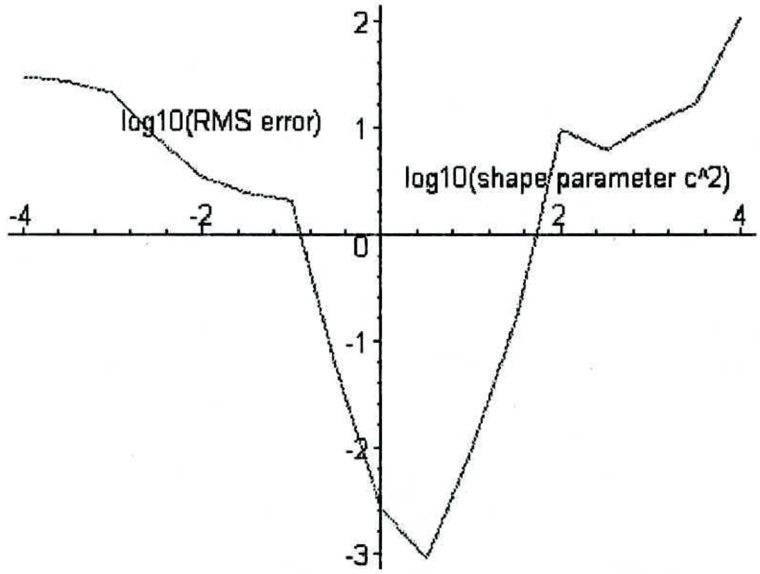

Figure 2.1.3 log(shape parameter c) vs log(RMSE) of function f3 interpolated over dataset S3using RMQ RBF.

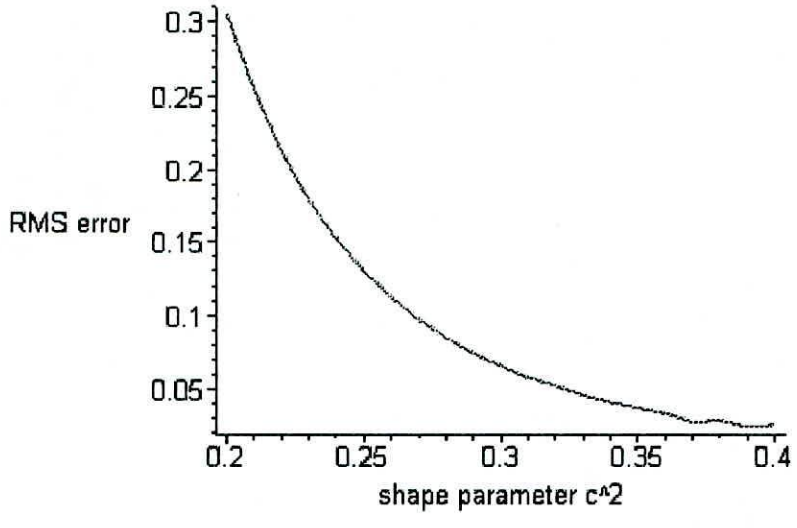

Figure 2.1.4 Shape parameter c vs RMSE of function f3 interpolated over dataset S3 using RMQ RBF.

When function f3 interpolated over dataset S3 using GA, we determined optimal1 c^2 as 3.1. However, due to numerical instability we were unable to approach this value and were only able to go as far as 0.35. So this 'break down' point is the optimal2 c^2 value. Beyond this the graph becomes unsmooth indicating instability (see Figure 2.1.3, 2.1.4). In few cases we got smooth curves with local minimum when fine-tuning c^2. In these cases, when optimal1 c^2 and optimal2 c^2 are nearly equal it can be seen that the optimal2 c^2 is a good approximation of optimal c^2. For example, when f2 interpolated over dataset S1 using MQ the values of optimal1 c^2, optimal2 c^2 are 10, 6.15 respectively (see Figure 2.1.1, 2.1.2).

In the RMSE table two RMS errors are given namely optimal1 c^2, optimal2 c^2. For optimal1 the order of the RMS error is given since in most cases optimal1 computation is unstable (see Appendix code A1.1.2).

As Rippa [11] has observed we also came to the same conclusion that optimal c^2 depends on the following factors:

1) Number of the data points.

2) Distribution of the data points.

3) Function approximated.

4) Precision of computation

Carlson and Foley [12] argued that optimal c^2 is essentially independent of the number and distribution of data points. By looking at the shape parameter c^2 table we can see that it might be true in some cases but not in many other. For example function f5 when interpolated over datasets S1, S3 using MQ RBF the optimall c^2 are 100, 10 respectively (see Table 2.1.1, 2.1.3). This indicates that optimal c^2 depends on number of data points.

When function f1 interpolated over datasets S5, S6 using RMQ RBF, we obtained optimall c^2 31.6, 3.1 respectively (see Table 2.1.5, 2.1.6). This shows that although datasets S5 and S6 have same number of data points their distribution has an effect on the optimal shape parameter.

Also both Carlson and Foley [12] observed that optimal c^2 is strongly depends on the function approximated, which confirms our observation. For the same dataset and RBF different functions have different optimal shape parameters (see Table 2.1.5).

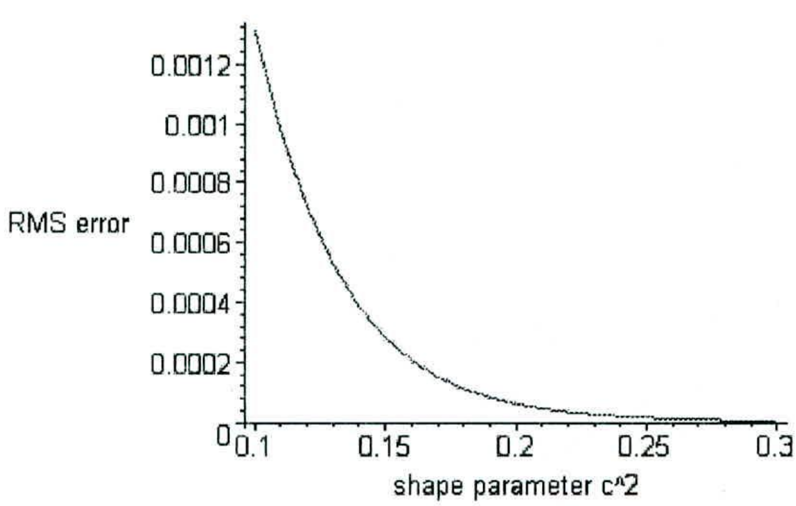

Figure 2.1.5 Shape parameter c^2 vs. RMSE of function f6 interpolated over dataset S3 using GA RBF drawn using 20 digits precision in Maple software.

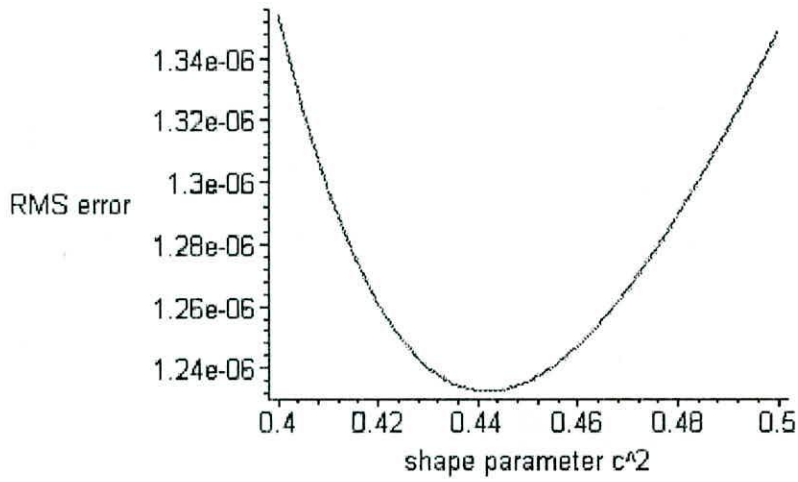

Figure 2.1.6 Shape parameter c^2 vs RMSE of function f6 interpolated over dataset S3 using GA RBF drawn using 25 digits precision in Maple software.

Now if we consider factor 4, all the computations in this document were carried out with 20 digits precision in Maple software. The precision of computation comes into play when we fine-tune c^2. For instance for function f6 interpolated over data set S3 the optimal2 c^2 is 0.3 (see Figure 2.1.4). Beyond that the computation is unstable. But when we do the computation in 25 digits precision optimal2 c^2 is 0.44 (see Figure 2.1.6). In our numerical experiments to find the 'optimal c^2' the following observations are made:

- For all three radial basis functions MQ, RMQ and GA the overall shape of the log (RMSE) versus log (shape parameter c^2) plot is essentially the same. The error seems decreasing down to a value of c^2 then increases sharply.
- In most cases, for the same function and dataset MQ and RMQ minimal error seem to occur for nearly the same c^2 values. This confirms the observation of

Carlson and Foley that optimal c^2 for both MQ and RMQ are nearly same (see Tables 2.1.5, 2.1.6).

- Compared to other two radial basis functions, for the same function and dataset the optimal c^2 for GA is relatively small. For function f1 interpolated over dataset S4 the optimal1 c^2 values for MQ, RMQ and GA RBF are 10.0,10.0,1.0 respectively (see Table 2.1.4).
- For the same function and radial basis function as the data points increase the optimal c^2 seems to get smaller. When function f3 interpolated over data sets S1, S3, S5 using MQ RBF the optimal1 c^2 are 31.6, 10.0, 3.1 respectively (see Tables 2.1.1, 2.1.3, 2.1.5)
- When the values of optimal1 c^2 and optimal2 c^2 are nearly equal then we can presume the optimal2 c^2 is a good approximation for real optimal c^2. Consider function f4 interpolated over dataset S4 using MQ RBF the values of optimal1 c^2 and optimal2 c^2 are 1.0, 0.96 respectively (see Table 2.1.4).

- When optimal1 c^2 is large we were unable to fine-tune c^2 and obtain good optimal2 c^2 because of severe ill-conditioning of matrix A. consider functions f1 and f5 interpolated over dataset S1 using MQ RBF whose optimal1 c^2 values are 316.0 and 100.0 (see Table 2.1.1).

Now we analyze the performance of various schemes mentioned above. The shape parameters obtained using these schemes are given in Tables 2.1.1-2.1.6 (see Appendix code A1.1.1).

- The error produced when using c^2 value obtained using Hardy's scheme [7] is unacceptable.

- Of all the schemes studied for MQ and RBQ interpolants Modified Franke's method 2 is the most promising method. Mod Fra1 is the second most effective method (see Tables 2.1.7, 2.1.8, 2.1.9 and Appendix B Tables 2.1.1-2.4.6)
- In some cases Frank and Foley [7] schemes perform equally well if not better. Consider function f8 interpolated over dataset S2 using RMQ RBF the RMSE error for Frank's and Foley's schemes are 1.6E-2, 7.1E-2 respectively which are of same order as that of Modified Frank [7] schemes (see Table 2.1.10).
- For GA radial basis function Frank's [7] scheme consistently produces good result than the other schemes (see Table 2.1.11).

  Despite the fact Modified Franke's method 2 consistently gives better c^2 values, in most cases they are greater than the optimal2 c^2 value, which in turn makes the computation of error unstable. One way to overcome this problem is to increase the precision of computation. Since cost of computation also increases with it, we can overcome this by developing robust algorithms to solve system of linear equations.

Fn	Frank c^2	Foley c^2	modFra1 c^2	modFra2 c^2	Optimal MQ c^2		Optimal RMQ c^2		Optimal GA c^2	
					1	2	1	2	1	2
1	.694	.198	1.875	8.33	316.0	15.0	316.0	26.0	100.0	6.0
2	.694	.198	1.875	8.33	10.0	15.0	10.0	7.4	1.0	1.04
3	.694	.198	1.875	8.33	31.6	18.0	31.6	23.0	10.0	7.0
4	.694	.198	1.875	8.33	1.0	1.2	1.0	1.38	0.31	0.28
5	.694	.198	1.875	8.33	100.0	17.0	100.0	20.0	3.1	7.50
6	.694	.198	1.875	8.33	31.6	14.5	31.6	18.0	3.1	3.24
7	.694	.198	1.875	8.33	100.0	17.0	100.0	23.0	31.6	8.50
8	.694	.198	1.875	8.33	31.6	12.0	1.0	0.95	1.0	0.48

Table2.1.1 Optimal shape parameters using MQ, RMQ and GA RBF and shape parameters obtained using schemes for 8 test functions interpolated over dataset S1.