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FINDING AN EFFECTIVE SHAPE PARAMETER STRATEGY TO OBTAIN THE OPTIMAL SHAPE PARAMETER OF THE OSCILLATORY RADIAL BASIS FUNCTION COLLOCATION IN 3D

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Abstract. Recent research into using the Method of Approximate Particular Solutions to numerically solve partial differential equations, has shown promising results. High levels of accuracy can be obtained when implementing this method, however the success of this collocation method is dependent on a shape parameter that is found in nearly all radial basis functions. If the shape parameter is not appropriately chosen, then it can provide an unacceptable result. Two shape parameter strategies are considered, a random variable shape parameter strategy and a leave-one-out cross validation strategy. The main objective of this work is to assess the viability of using these shape parameter strategies with oscillatory radial basis function, and their ability to provide a consistent and accurate approximation.

Keywords: *Numerical solutions of partial differential equations, Oscillatory radial basis functions*

MSC (2010): Primary 65N35

1. Introduction

Consider the following time independent, linear, elliptic partial differential equations (PDEs) in 3D:

$$\begin{aligned} \mathcal{L}u &= f(\mathbf{x}),\ \mathbf{x} \in \Omega, \\ \mathcal{B}u &= g(\mathbf{x}),\ \mathbf{x} \in \partial\Omega, \end{aligned} \tag{1.1}$$

where $\mathcal{L}$ is the linear differential operator, and $\mathcal{B}$ the boundary differential operator. The interior of the domain is defined by Ω, the boundary of the domain by $\partial\Omega$, $\mathbf{x} = (x, y, z)$ is a point in 3D, and u is the analytical solution of (1.1).

Several numerical methods have been proposed throughout the history to obtain the numerical solutions of different PDEs. Among these, Method of Approximate Particular Solutions (MAPS) is one of the meshless numerical methods proposed by Chen et al [1] to solve PDEs. MAPS is a collocation based method which assumes that the solution u of the PDEs can be approximated by the linear superposition of the particular solutions. So, to apply MAPS, we assume that

$$u \approx \sum_{i=1}^{n} a_i \Phi_i(\mathbf{x}), \tag{1.2}$$

where a_i are the unknown coefficients to be determined, and Φ_i are the particular solutions based basis functions. If we choose the basis functions to be radial basis functions (RBFs), then Φ_i can be constructed as follows:

$$\Phi_i(\mathbf{x}) = \Phi\left(||\mathbf{x} - \mathbf{x_i}||\right), \tag{1.3}$$

where $||\mathbf{x}-\mathbf{x_i}||$ is the euclidean distance between $\mathbf{x}$ to $\mathbf{x_i}$, $i=1,2,...,n$, computational nodes. Using Eq. (1.2), and (1.3), we obtain

$$u \approx \sum_{i=1}^{n} a_i \Phi\left(||\mathbf{x}-\mathbf{x_i}||\right). \tag{1.4}$$

Applying Eq. (1.4) to Eq. (1.1) with n_i interior computational nodes $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_{n_i}$, and n_b boundary computation nodes $\mathbf{x}_{n_i+1}, \mathbf{x}_{n_i+2}, ..., \mathbf{x}_{n_i+n_b}$, produces the $n = n_i + n_b$ system of equations as:

$$\begin{aligned} \sum_{i=1}^{n} a_i \mathcal{L}\Phi\left(||\mathbf{x_j}-\mathbf{x_i}||\right) &= f(\mathbf{x_j}) \quad j=1,2,...,n_i, \\ \sum_{i=1}^{n} a_i \mathcal{B}\Phi\left(||\mathbf{x_j}-\mathbf{x_i}||\right) &= g(\mathbf{x_j}) \quad j=n_i+1, n_i+2, ..., n_i+n_b. \end{aligned} \tag{1.5}$$

These systems of equations (1.5) can be written in the matrix form as

$$\mathbf{A}\alpha = \mathbf{F}, \tag{1.6}$$

where $\mathbf{A}$ is the interpolant matrix, α needs to be computed as it contains undetermined coefficients as its components, and $\mathbf{F}$ is the right hand side vector.

The particular solution Φ can be obtained by the relation

$$\Delta\Phi = \phi,$$

where ϕ is a RBF. In this project, we have chosen the ϕ as one of the following oscillatory radial basis functions (O-RBFs)

$$\phi_n(r) = \frac{J_{n-1/2}(cr)}{(cr)^{n-1/2}},$$

where J_μ is the Bessel function of the first kind of order μ, $c>0$ is a constant shape parameter, and r is the radial distance in 3-space. Note that, for $n=0,1,2...$, these O-RBFs can be written as

$$\begin{aligned} \phi_0(r) &= \sqrt{\frac{2}{\pi}}\cos(cr), \\ \phi_1(r) &= \sqrt{\frac{2}{\pi}}\frac{\sin(cr)}{cr}, \\ \phi_2(r) &= \sqrt{\frac{2}{\pi}}\left(\frac{\sin(cr)}{c^3r^3} - \frac{\cos(cr)}{c^2r^2}\right). \end{aligned}$$

In [4], Manns et al have derived the particular solutions based basis function Φ corresponding to ϕ_1. Using the similar derivation, the Φ corresponding to ϕ_2 can be obtained as

$$\Phi(r) = -\sqrt{\frac{2}{\pi}}\frac{\mathrm{Si}(cr)}{c^3 r}, \tag{1.7}$$

where Si is the sine integral.

We observe that the RBFs, and the particular solutions based basis functions include the shape parameter. The accuracy of the numerical solutions relies heavily on the shape parameter. In this project, we focus on choosing an optimal shape parameter that improves the numerical accuracy. In Sections 2 and 3, we discuss the two strategies which we have adopted in this project. Numerical examples are presented in Section 4, and conclusion of the project is given in Section 5.

2. Random Variable Shape Parameter Strategy

Researchers have often speculated that a variable shape parameter strategy would be effective in providing a minimal error in approximation. When discussing a variable shape parameter, it is the idea of having the possibility for a different shape parameter value to be used at each of our collocation points. The complexity that is added to an already complex and nuanced problem is notable and this has led to a lack of widespread research into the strategy until recently. Variable shape parameter strategies provide better approximations due to being able to better fit extreme variations or steep gradients that can be found in functions. In this work, we will focus on random variable shape parameters as defined by [6]

$$c_i = c_{min} + (c_{max} - c_{min}) \times \text{rand}(1, n), \tag{2.1}$$

where $c = (c_1,\ c_2,\ c_3,\ ...\ c_n)$ is the variable shape parameter with the given bounds (c_{min}, c_{max}), and $\text{rand}(1, n)$ are the n random numbers in $(0, 1)$. Some advantages of the random variable shape parameter come from it not universally increasing or decreasing. Other variable shape parameter strategies such as a linear variable strategy, will have relatively large values found at the end of the interval, which can lead to a degradation of the approximation. The random variable shape strategy is able to avoid this degradation and provide an optimal approximation [6].

Once we select the random variable shape parameters $c = (c_1,\ c_2,\ c_3,\ ...,\ c_n)$ from Eq. (2.1), Eq. (1.2) can be written as

$$u \approx \sum_{i=1}^{n} a_i \Phi(||\mathbf{x} - \mathbf{x_i}||, c_i). \tag{2.2}$$

With this new variable added to the summation it is important to associate that $c_1,\ c_2,\ c_3,\ ...,\ c_n$ iterates along with the summation of the different collocation points. Thus giving the possibility for unique shape parameters at each point.

3. Leave-One-Out Cross Validation

As stated by Fasshauer [2], there are many cross validation strategies that are well-known in statistics literature. Some of the more popular strategies of cross validation include the k-fold cross validation strategy, along with the validation set approach. These algorithms are known to minimize a cost function to provide an optimal shape parameter. As Rippa has stated [5], using leave-one-out cross validation (LOOCV) is an attempt to take the number and distribution of data points and the precision of computation into account to most accurately represent PDEs. To apply LOOCV, for $k = 1, 2, ..., n$, we will create a set $\mathbf{X_{[k]}}$ consisting of all nodes except $\mathbf{x_k}$:

$$\mathbf{X_{[k]}} = \{\mathbf{x_1}, \mathbf{x_2}, ..., \mathbf{x_{k-1}}, \mathbf{x_{k+1}}, ..., \mathbf{x_n}\}.$$

Using the nodes from this set, we solve the $n - 1$ system of equations in Eq. (1.5) to obtain the vector $\alpha_{[\mathbf{k}]} = a_{i_{[k]}}$, consisting of corresponding undetermined coefficients. Finally, we can create an error vector $\mathbf{E}$, that consists of error values

$$e_k = \begin{bmatrix} f(\mathbf{x_k}) - \sum_{i=1}^{n} a_{i_{[k]}} \mathcal{L}\Phi\left(||\mathbf{x_k} - \mathbf{x_i}||\right) \\ \\ g(\mathbf{x_k}) - \sum_{i=1}^{n} a_{i_{[k]}} \mathcal{B}\Phi\left(||\mathbf{x_k} - \mathbf{x_i}||\right) \end{bmatrix}.$$

Minimizing this error vector determines the overall fit to the entire data set, and serves as a cost function to assist in returning the appropriate shape parameter. An improved method of finding the

error associated with each interpolant was proposed by Rippa [5]. It is shown that Rippa's formula is a rather cheaper algorithm, given by

$$e_k = \frac{a_k}{A^{-1}_{kk}},$$

where A^{-1}_{kk} is the $k-$th diagonal element of the inverse matrix of A of Eq. (1.6).

4. Numerical Examples

The goal of the numerical examples, as stated above, is to minimize the error of approximation through finding the optimal shape parameter. We will be presenting numerical solutions of two Poisson's Equations with the help of the particular solutions obtained in Eq. (1.7). To check the numerical accuracy we have used the Root Mean Square Error (RMSE) which is defined by,

$$\text{RMSE} = \sqrt{\frac{1}{n_t}\sum_{j=1}^{n_t}(\hat{u_j} - u_j)^2}, \tag{4.1}$$

where u_j representing the solution at the jth node, $\hat{u_j}$ is the approximate solution obtained by MAPS, and n_t representing the number of test points. Numerical examples are conducted over an unit cube domain with 1000 interior and 728 boundary points.

Example 1: Consider Eq. (1.1) with $\mathcal{L} := \Delta$, Δ is the Laplace Operator, $\mathcal{B} := I$, I is the identity operator, and

$$\begin{aligned} f(x,y,z) &= -3\cos(x)\cos(y)\cos(z) \\ g(x,y,z) &= \cos(x)\cos(y)\cos(z). \end{aligned}$$

In Figure 1, we observe that the numerical accuracy of the MAPS depends on the shape parameter. Note that the plot is obtained by choosing the constant shape parameter.

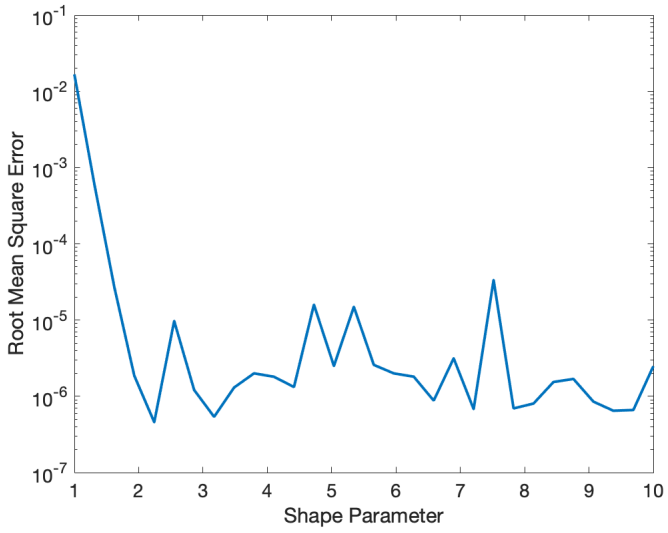

Figure 1. Example 1: Shape parameter vs Root Mean Square Error plot

Table 4.1 shows that using the random variable shape parameter, we would achieve far more accurate solution than obtained from the constant shape parameter.

For random variable shape parameter strategy, each approximation there is a certain amount of variation due to the random number generation for the approximation, knowing that each test is run multiple times in an attempt to get a representative interval for there error. The Min and Max error shown in the table is the lowest and the highest RMSE achieved through the testing.

Interval	Min RMSE	Max RMSE
(3,8)	7.8155E-12	5.5166E-11
(1,10)	1.6121E-11	6.1932E-11
(1,5)	2.6238E-10	9.6585E-09
(5,10)	6.7370E-11	5.1915E-10

Table 4.1. Example 1: Root Mean Square Error Obtained by random variable shape parameter strategy

Interval	Optimal c value	RMSE
(0,10)	7.645887	7.04E-07
(3,8)	5.983739	1.10E-06
(1,10)	8.826156	3.84E-07
(1,5)	2.975109	3.20E-07
(5,10)	6.157643	4.29E-07

Table 4.2. Example 1: Root Mean Square Error Obtained by leave-one-out cross validation strategy

On the other hand, Table 4.2 shows that LOOCV strategy is effective on capturing the appropriate constant shape parameter. Due to the local minimization function involved in minimizing the error vector, we have presented the results by choosing different intervals as initial guess.

Example 2: Again, consider equation (1.1) with $\mathcal{L} := \Delta$, Δ is the Laplace Operator, $\mathcal{B} := I$, I is the identity operator, and

$$\begin{aligned} f(x,y,z) &= 3e^{(x+y+z)} \\ g(x,y,z) &= e^{(x+y+z)}. \end{aligned}$$

Interval	Min RMSE	Max RMSE
(3, 8)	2.7819E-10	1.8024E-09
(1, 10)	7.2946E-10	1.8398E-09
(1, 5)	7.9333E-09	3.4988E-07
(5, 10)	5.1525E-09	8.7261E-07

Table 4.3. Example 2: Root Mean Square Error Obtained by random variable shape parameter strategy

As can be seen in the tables above, the random variable shape parameter provided a more accurate approximation that LOOCV does. It is important to note that LOOCV provide us the appropriate shape parameter after solving the system. On the other hand, the shape parameters on random variable shape parameter are pre-determined (randomly) by the Eq. (2.1).

Interval	Optimal c value	RMSE
(0, 10)	7.808969	5.22E-05
(3, 8)	5.343108	7.35E-05
(1, 10)	7.341710	7.30E-05
(1, 5)	3.067396	8.28E-04
(5, 10)	8.317156	4.64E-05

Table 4.4. Example 2: Root Mean Square Error Obtained by leave-one-out cross validation strategy

5. Conclusion

In conclusion, the data shown suggests that random variable shape parameter strategy and the LOOCV are able to effectively find an optimal shape parameter. The testing shows random variable shape parameter providing less error when approximating then LOOCV. Its important to note that the numerical examples shown here are only conducted on one type of PDEs, so further test results are necessary for any broad conclusions to be made about which method leads to better approximations. Nevertheless, the results of our tests are encouraging that these strategies could potentially provide a more efficient and effective way to numerically solve the PDEs in the future.

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