Improved Numerical Approach for the Kansa's Method

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March 10, 2004

Abstract

Radial Basis functions (RBFs) have been successfully developed as a truly mesh-less method to find the numerical solutions of partial differential equations (PDEs). In particular, the asymmetric RBF collocation method (Kansa's method) is one of the most frequently used methods due to its ease of implementation. To achieve high accuracy, the resultant system of RBF-PDE problem usually becomes badly conditioned. We propose in this paper an improved solution method based on an affine space decomposition that decouples the influence between the interior and boundary collocations.

1 Introduction

The original idea of the RBFs is to interpolate scattered data $\{\vec{x}_k, f(\vec{x}_k)\}$ for $k = 1, \ldots, N$ by using the function space span$\{\phi(r_k) : \ k = 1, \ldots, N\}$ where ϕ is any radial basis function and $r_k = \|\vec{x} - \vec{x}_k\|_2$ denotes the Euclidean distance between the variable $\vec{x}$ and the centers $\vec{x}_k$. All these RBFs can be scaled by a simple transform $r_k \leftarrow \dfrac{r_k}{c}$ where c is referred as the shape parameter.

Previous authors have observed experimentally that the accuracy of RBF methods is severely influenced by the shape parameter c and the separating distance h of the centers. The trade-off for this increased accuracy and ill-conditioning of the associated linear systems can be explained by the "uncertainty relation" given by Schaback [8, 9, 10]. Despite of its superior convergence properties, the mesh-less RBF methods have not been applied at present to large-scale PDE simulations. One of the main reasons is that both the global and compactly supported RBFs give rise to either very large full matrices, or large wide-banded matrices that are known to be severely ill-conditioned. The optimal convergence in using the compact support RBFs occurs as the support becomes increasingly more global unless a multilevel scheme is invoked.

To solve RBF-PDE systems on a fixed arithmetic precision (floating point relative accuracy, i.e., the commonly used *double precision*), the problem of

ill-conditioning and rounding error will eventually have great impact on the accuracy. For numerical verifications, we focus in this paper upon the asymmetric formulation (Kansa's method [4, 5]) for solving PDEs with MQ-RBF as its conditioning and accuracy can be greatly affected by the shape parameter c. On the other hand, our proposed method can be extended to other RBFs directly. A main goal of this paper is to provide a new numerical scheme that

1. is *easy* to implement,
2. is *efficient* comparing with existing methods,
3. have a *larger* critical shape parameter,
4. is *stable* for large shape parameters beyond critical, and
5. does *not* require *distinct* data points distribution.

The outline of this paper is as follows: in Section 2, the Kansa's asymmetric RBF-PDE formulation is reviewed. In Section 3, the affine space approach is introduced. Summary of results are given in Section 4. Lastly, the conclusion is given in Section 5. Analysis and numerical results are left to a forthcoming paper.

2 Asymmetric RBF-PDE Method

Consider the boundary value problems (BVPs) of the form

$$\begin{array}{rcll} \mathcal{L}u & = & f(\vec{x}) & \text{in } \Omega \subset \mathbb{R}^d, \\ \mathcal{B}u & = & g(\vec{x}) & \text{on } \partial\Omega, \end{array} \tag{1}$$

where d denotes the spatial dimension, $\partial\Omega$ denotes the boundary of the domain Ω, $\mathcal{L}$ is an interior differential operator, and $\mathcal{B}$ is an operator that specifies the boundary conditions of Dirichlet, Neumann or mixed type. Both f and g are given functions mapping $\mathbb{R}^d \to \mathbb{R}$.

In Kansa's asymmetric RBF collocation method, the unknown solution u of (2) is approximated by a linear combination of RBFs in the form of

$$u \approx U(\vec{x}) = \sum_{k=1}^{N} \lambda_k \, \phi_k(\vec{x}), \tag{2}$$

where $\phi_k(\vec{x}) = \phi(\|\vec{x} - \vec{x}_k\|)$, $\phi(\cdot)$ is any radial basis function, and $\|\cdot\|$ indicates the Euclidean norm. Let $\{\vec{x}_j\}_{j=1}^{N}$ be the N centers and collocation points in $\Omega \cup \partial\Omega$. We assume the centers are arranged in such a way that the first N_I points and the last N_B points are in Ω and on $\partial\Omega$, respectively.

Using collocation method to ensure that $U(\vec{x})$ satisfies (1), we obtain a numerical approximation of u. To solve for the N unknown coefficients $\vec{\lambda} =$

$[\lambda_1, \ldots, \lambda_N]^T$ in (2), we need to solve the following N (hopefully) linearly independent equations. In matrix form, we have the *resultant system* given by

$$\begin{bmatrix} \Phi_{\mathcal{L}} \\ \Phi_{\mathcal{B}} \end{bmatrix} \vec{\lambda} = \begin{bmatrix} \vec{f} \\ \vec{g} \end{bmatrix}, \qquad \text{or} \qquad \Phi\vec{\lambda} = \vec{b}, \tag{3}$$

where $\vec{f} \in \mathbb{R}^{N_I}$, $\vec{g} \in \mathbb{R}^{N_B}$, $\Phi_{\mathcal{L}} \in \mathbb{R}^{N_I \times N}$, $\Phi_{\mathcal{B}} \in \mathbb{R}^{N_B \times N}$, and

$$\begin{array}{rcll} (\vec{f})_i & = & f(\vec{x}_i), & \text{for } i = 1, \ldots, N_I, \\ (\vec{g})_i & = & g(\vec{x}_i), & \text{for } i = 1, \ldots, N_B, \\ (\Phi_{\mathcal{L}})_{ik} & = & \mathcal{L}\phi(\vec{x}_i - \vec{x}_k), & \text{for } i = 1, \ldots, N_I,\ k = 1, \ldots, N, \\ (\Phi_{\mathcal{B}})_{ik} & = & \mathcal{B}\phi(\vec{x}_i - \vec{x}_k), & \text{for } i = N_I + 1, \ldots, N,\ k = 1, \ldots, N. \end{array} \tag{4}$$

This method is often named as asymmetric RBF collocation method or Kansa's method. The matrix given by (3) is generally non-symmetric and full. This resultant system is known to be ill-conditioned when N becomes large.

Unlike the interpolation problems, the Kansa's method could result in singular resultant matrix for some special centers arrangements. Experimental evidence (see Hon and Schaback [3]) indicates that the Kansa's method is robust with regard to the positioning of centers with a general prerequisite that all centers are distinct.

When $\frac{c}{h}$ is fixed at a low ratio, the resulting linear system remains *relatively well-conditioned* (condition number of the problem is significantly less than the inverse of machine epsilon). This is the case on which different preconditioning techniques can be employed; see Beatson et al.[1, 2] for interpolation problems and Ling et al.[6, 7] for PDE problems. To take the full advantage of RBF superior convergence rate, one must keep increasing the $\frac{c}{h}$ ratio. For any given arithmetic precision and solution method, there exists a (numerical) "critical" shape parameter c^* after which the rounding error becomes substantial and the numerical approximation is no longer trustworthy.

3 Affine Space Approach

The matrix Φ in the resultant system (3) consists of two parts: the interior collocation matrix $\Phi_{\mathcal{L}}$ and the boundary collocation matrix $\Phi_{\mathcal{B}}$, resulting from the interior operator $\mathcal{L}$ and boundary operators $\mathcal{B}$, respectively. It has been observed by many authors that combining these matrices with different "length scales" usually worsens the problem of ill-conditioning (comparing with the interpolation problems). In this section, we proposed an affine space approach aimed to circumvent the above problem. The RBF unknown coefficient vector $\vec{\lambda}$ is decomposed by the orthonormal basis of the null space of $\Phi_{\mathcal{B}}$. We then obtain a better conditioned reduced matrix system for the new coefficient vector.

From (3), we know the unknown coefficients $\vec{\lambda}$ must satisfy $\Phi_{\mathcal{B}}\vec{\lambda} = \vec{g}$. This suggests the coefficient vector $\vec{\lambda}$ must lie in an affine space of $\mathcal{N}_{\mathcal{B}}$, namely

$$\vec{\lambda} = \Phi_{\mathcal{B}}^{\dagger}\vec{g} + \mathcal{N}_{\mathcal{B}}\vec{\gamma}, \tag{5}$$

where $\Phi_{\mathcal{B}}^{\dagger} \in \mathbb{R}^{N \times N_B}$ is the pseudoinverse of $\Phi_{\mathcal{B}}$ and $\mathcal{N}_{\mathcal{B}} \in \mathbb{R}^{N \times N_I}$ is the null space matrix of $\Phi_{\mathcal{B}}$. Both matrices, $\Phi_{\mathcal{B}}^{\dagger}$ and $\mathcal{N}_{\mathcal{B}}$, can be obtained from the SVD of $\Phi_{\mathcal{B}}$. Putting (5) into the interior PDE portion of (3) given by $\Phi_{\mathcal{L}}\vec{\lambda} = \vec{f}$, results in the following *reduced system* to solve for another unknown coefficient vector $\vec{\gamma} \in \mathbb{R}^{N_I}$,

$$(\Phi_{\mathcal{L}}\mathcal{N}_{\mathcal{B}})\vec{\gamma} = \vec{f} - \Phi_{\mathcal{L}}\Phi_{\mathcal{B}}^{\dagger}\vec{g}, \tag{6}$$

where the reduced matrix $(\Phi_{\mathcal{L}}\mathcal{N}_{\mathcal{B}}) \in \mathbb{R}^{N_I \times N_I}$ is a square matrix. Since $\mathcal{N}_{\mathcal{B}}$ is orthogonal, the length scale of the reduced matrix in (6) is completely determined by the PDE interior operator $\mathcal{L}$. The original RBF-PDE systems (3) and the affine space approach (5)+(6) are mathematically identical. However, due to the presence of ill-conditioning and rounding error, the matrices and vectors dimensions found in (5)+(6) could vary in practices.

As the $\frac{c}{h}$ ratio increases and as the RBF-PDE matrices become ill-conditioned, any singular values of $\Phi_{\mathcal{B}}$ less than a default tolerance are treated as zero numerically (although the matrix could still be mathematically full rank). As a result, the null space matrix $\mathcal{N}_{\mathcal{B}}$ will be of size $N \times (N - M)$, where $M := \text{rank}_{SVD}(\Phi_{\mathcal{B}}) < N_B$ and $N - M$ is the nullity of $\Phi_{\mathcal{B}}$. Consequently, the reduced matrix is no longer square but of size $N_I \times (N - M)$. Since $N - M > N_I$, the reduced system (6) is underdetermined and the new unknown coefficient vector $\vec{\gamma}$ is of length $N - M$. Furthermore, the reduced matrix could also be rank deficient, i.e., $\text{rank}_{SVD}(\Phi_{\mathcal{L}}\mathcal{N}_{\mathcal{B}}) < N - M$. Without assuming the system is of full-rank, the reduced system (6) is solved by either QR or SVD (abbreviated by AQR and ASVD, respectively) for the new coefficient vector $\vec{\gamma}$.

In the traditional Kansa's method, extra work is needed to ensure all centers are distinct, and ideally to ensure the minimum separating distances among the centers are equal in magnitude. The fact that our proposed algorithm can handle identical or extremely close centers gives extra flexibility to the mesh-less RBF methods.

4 Results

The GE method is the fastest solver for all N; whereas SVD and ASVD are the most time consuming methods as the singular value decompositions of full matrices are required. The CPU times used for setting up the affine space methods are roughly the same as the *QR-time* since SVD is only applied to a much smaller matrix $\mathcal{N}_{\mathcal{B}}$. Since the reduced system (6) is of smaller size comparing with the resultant system (3), we see that *AQR-time* < *QR-time*. It is worth noting that the Matlab's function *MLDIVIDE* (our reported *GE-time*) is optimized for nonsingular square matrices (using Matlab's function *LU* to preform the same Gaussian eliminations would only take slightly fewer CPU time than our reported *QR-time*). We compare these methods as follows:

GE: The method is the best direct method in terms of efficiency and accuracy although it could be unstable for ill-conditioned systems. The limitation is that the GE method cannot be used on singular formulations.

QR: The method are not recommended for all cases due to its extreme instability for ill-conditioned problems and is costly compared with GE.

SVD: The most costly method that does not result in the best accuracy. On the other hand, this is the only direct method that is suitable for extremely ill-conditioned systems and singular formulations.

AQR: The method is able to handle ill-conditioned system and achieve higher accurate results with a reasonable cost. The AQR method also allows singular formulation that further simplify the setup of some PDE problems.

ASVD: The method is similar to AQR in performance, but needs a much higher cost and is not recommended for practical problems.

To sum up, the GE method is still the best choice for well-conditioned RBF-PDE systems. To take full advantage of the spectral convergence of RBFs, the AQR method should be employed. Although some direct methods can handle singular formulations, they all have their own drawbacks. Our proposed AQR method is much more flexible and make the setup of Kansa's method easier than ever.

5 Conclusion

We propose an affine space approach for improving the Kansa's method. Our method decouples the influence between the interior and boundary collocations, is easy to implement, and is able to achieve better accuracy. The method used in this paper allows the use of larger RBF shape parameter. Comparing with different direct approaches, the extra work of our method can be compensated when the same accuracy is obtained by a smaller number of data points. The proposed method can also be benefit from the previous work of domain decomposition.

On the other hand, it requires further development and the numerical experiments reported here should only be considered as exploratory work. More work is needed to further verify the numerical observations and to find a robust numerical scheme.

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