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Short Communication

Mathematical justification for RBF-MFS

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Abstract

In this note, we revisit the RBF-MFS which couples Kansa's technique with the method of fundamental solution (MFS). The idea of RBF-MFS was originally proposed by Golberg in 1995 and used by many engineers later, but the solvability of this method is never justified mathematically. Here we prove that RBF-MFS is theoretically solvable for Hardy's multiquadrics and the cubic radial basis function for the Poisson operator. Numerical results show that the RBF-MFS is comparable to Kansa's method. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Radial basis function; Collocation method; Dual reciprocity method; Method of fundamental solution; Kansa's method

1. Introduction

Since the pioneering work of Kansa [1] on solving partial differential equations (PDEs) by collocation using radial basis functions (RBFs) in 1990, such technique (named as Kansa's method by Golberg and Chen [2]) has been applied successfully to the numerical solutions of various type of ordinary and partial differential equations including the biphasic mixture model for tissue engineering problems [3], heat transfer [4], 1-D nonlinear Burgers' equation [5], shallow water equation for tide and currents simulation [6,7], and free boundary problems arising in American option pricing [8,9] and in steady solid–liquid phase-change systems [10].

In general, Kansa's method has several advantages over the widely used finite element methods (FEM) and finite volume methods (FVM) in that:

1. Kansa's method is truly meshless in which the collocation points can be chosen freely (no connectivity between points is required as FEM and FVM). Hence, the complicated meshing problem for FEM and FVM has been avoided.
2. While Kansa's method shares the same wide range of applicability as FEM and FVM, the implementation of Kansa's method is much simpler compared to FEM and FVM, and the superior convergence of Kansa's method has been observed.

Despite these advantages, the proof of nonsingularity of the linear system resulting from Kansa's method was still unavailable. Though Schaback and Hon [11] recently showed that a general proof of this fact is practically impossible through some numerical experiments.

Another type of meshless method with RBFs is the classic MFS-DRM, which is evolved from the dual reciprocity boundary element method (DRBEM) [12]. In the MFS-DRM, the method of fundamental solutions (MFS) has been used instead of boundary element method (BEM) in the process of the DRBEM. Details about MFS can be found in the excellent review papers [13,14]. Details about DRBEM can be found in the classic book [15]. Most recent results related to MFS-DRM are provided in Refs. [14,16,17]. Note that in the classic MFS-DRM, the RBFs are used for the approximation of the right-hand side function of the equation so that an analytical particular solution can be found, which is not a trivial task for differential operators other than Laplacian or bi-harmonic [14]. Several methods for approximating particular solutions have been presented in the literature [18–24]. More details can be found in the review paper of Golberg [25]. In 1995, Golberg [25, p. 102] proposed a technique of evaluating the approximate particular solution by collocation using RBFs only for the differential equation (instead of collocation for both the differential equation and boundary conditions in Kansa's method). For convenience, we name this technique as RBF-MFS in the rest of the paper. We like to remark that RBF-MFS was restated in the book of Golberg and Chen [16, p. 323]. Similar ad-hoc approaches were proposed

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independently by various researchers in the BEM community. Among them, Chen and Tanaka [26] used multiquadric RBF $\varphi(r) = (r^2 + c^2)^{3/2}$ and Kögl and Gaul [27] used RBF $\varphi(r) = r^2 + r^3$ in their applications, respectively. However, no mathematical justification has been given before. Here we prove that theorectically RBF-MFS is solvable for Hardy's multiquadric $\varphi(r) = (r^2 + c^2)^{1/2}$ and the cubic radial basis $\varphi(r) = r^3$ for the Poisson operator.

The paper is organized as follows. In Section 2 we give a brief introduction to Kansa's method. Then in Section 3, we revisit RBF-MFS, which is proven to be theorectically solvable. Numerical results are presented to show that RBF-MFS achieves comparable results as Kansa's method. Conclusions are given in Section 4.

2. The Kansa's method

The Kansa's method was introduced in 1990 [1] for solving PDEs by collocation using radial basis functions. This technique is very general, simple and effective. It has been successfully applied in many different areas as we mentioned in Section 1.

Consider a general differential equation

$$Lu = f(x, y) \text{ in } \Omega, \qquad Bu = g(x, y) \text{ on } \partial\Omega, \tag{1}$$

where L is an arbitrary differential operator, B is an operator imposed as boundary conditions, such as Dirichlet, Neumann, and Robin.

Let us denote $\{P_i = (x_i, y_i)\}_{i=1}^N$ to be N collocation points in Ω of which $\{(x_i, y_i)\}_{i=1}^{N_I}$, are interior points; $\{(x_i, y_i)\}_{i=N_I+1}^N$ are boundary points. In Kansa's method, it is assumed that the approximate solution for problem (1) can be expressed as

$$u(x, y) = \sum_{j=1}^N u_j \varphi_j(x, y), \tag{2}$$

where $\{u_j\}_{j=1}^N$ are the unknown coefficients to be determined, and $\varphi_j(x, y) = \varphi(\|P - P_j\|)$ is a RBF. Here $r = \|P - P_j\|$ is the Euclidean norm between points $P = (x, y)$ and $P_j = (x_i, y_j)$. Most widely used radial basis functions are the multiquadric (MQ) $\varphi(r) = (r^2 + c^2)^{\beta/2}$ (β is an odd integer), the Gaussians (GS) $\varphi(r) = \mathrm{e}^{-cr^2}$, and the polyharmonic splines $\varphi(r) = r^{2n} \log r$ in $\mathscr{R}^2$ for $n \geq 1$ (thin plate splines for $n = 1$). We refer readers to the good review paper on the theory of RBF interpolation by Powell [28].

By substituting Eq. (2) into Eq. (1), we have

$$\sum_{j=1}^N (L\varphi_j)(x_i, y_i) u_j = f(x_i, y_i), \qquad i = 1, 2, \ldots, N_I, \tag{3}$$

$$\sum_{j=1}^N (B\varphi_j)(x_i, y_i) u_j = g(x_i, y_i), \qquad i = N_I + 1, N_I + 2, \ldots, N. \tag{4}$$

Hence we have to solve the following $N \times N$ linear algebraic system

$$\begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} \begin{bmatrix} u^{(1)} \\ u^{(2)} \end{bmatrix} = \begin{bmatrix} \mathbf{f}^{(1)} \\ \mathbf{f}^{(2)} \end{bmatrix}$$

for the unknowns $u^{(1)} = [u_1, \ldots, u_{N_I}]^{\mathrm{T}}$, $u^{(2)} = [u_{N_I+1}, \ldots, u_N]^{\mathrm{T}}$. Then the approximate solution can be obtained from Eq. (2) at any point in the domain Ω. Here we denote the submatries

$\mathbf{A}_{11}$ with element $(L\varphi_j)(x_i, y_i)$, $i, j = 1, 2, \ldots, N_I$,
$\mathbf{A}_{12}$ with element $(L\varphi_j)(x_i, y_i)$, $i = 1, 2, \ldots, N_I$, $j = N_I + 1, \ldots, N$,
$\mathbf{A}_{21}$ with element $(B\varphi_j)(x_i, y_i)$, $i = N_I + 1, \ldots, N$, $j = 1, 2, \ldots, N_I$,
$\mathbf{A}_{22}$ with element $(B\varphi_j)(x_i, y_i)$, $i = N_I + 1, \ldots, N$, $j = N_I + 1, \ldots, N$,

and vectors

$$\mathbf{f}^{(1)} = [f(x_1, y_1), f(x_2, y_2), \ldots, f(x_{N_I}, y_{N_I})]^{\mathrm{T}},$$
$$\mathbf{f}^{(2)} = [g(x_{N_I+1}, y_{N_I+1}), g(x_{N_I+2}, y_{N_I+2}), \ldots, g(x_N, y_N)]^{\mathrm{T}}.$$

From above, we can see that the implementation of Kansa's method is simple and direct. These are the main reasons that this technique is getting popular and has been applied to many areas [3–6,8–10]. However, the proof of the solvability (or nonsingularity) for the linear system resulting from Kansa's method is still unconfirmed yet, even for elliptic problems.

3. The MFS-DRM

The key ingredient in MFS-DRM for solving various linear PDEs $Lu = f$ is that we assume that the solution can be decomposed as $u = u_{\mathrm{p}} + v$, where u_{p} is the particular solution of $Lu = f$ without imposing any boundary conditions, v satisifies the homogeneous PDEs $Lv = 0$ with boundary conditions involving the obtained particular solution u_{p}.

3.1. The classic DRM

In the classic DRM, we first approximate the right-hand side function f by RBFs as

$$f_N(x) = \sum_{j=1}^N a_j \varphi(\|x - x_j\|) + \sum_{k=1}^l b_k p_k(x),$$

where $\varphi(\|x - x_j\|) : \mathscr{R}^d \to \mathscr{R}^+$ is a RBF, $\{p_k\}_{k=1}^l$ is the complete basis for d-variate polynomials of degree $\leq m - 1$, and C_{m+d-1}^d is the dimension of P_{m-1} [30]. The coefficients $\{a_j\}$, $\{b_k\}$ can be found by solving the system

$$\sum_{j=1}^N a_j \varphi(\|x_i - x_j\|) + \sum_{k=1}^l b_k p_k(x_i) = f(x_i), \qquad 1 \leq i \leq N,$$

$$\sum_{j=1}^{N} a_j p_k(x_j) = 0, \qquad 1 \le k \le l,$$

where $\{x_i\}_{i=1}^{N}$ are the collocation points on $\Omega \cup \partial\Omega$.

After obtaining the coefficients $\{a_j\}$, $\{b_k\}$, then the approximate particular solution $\hat{u}_p$ can be obtained by linearity

$$\hat{u}_p = \sum_{j=1}^{N} a_j \Phi_j + \sum_{k=1}^{l} b_k \Psi_k,$$

where

$$L\Phi_j = \varphi_j, \qquad \text{for } j = 1, \dots, N,$$

$$L\Psi_k = p_k, \qquad \text{for } k = 1, \dots, l.$$

Note that Ψ_k can be obtained by the method of undetermined coefficients, while the determination of Φ_j is not trivial [16,31,32].

3.2. The MFS

Note that the homogeneous problem for v can be solved by various boundary methods such as the method of fundamental solutions (MFS) [13,16]. The idea of MFS is to look for solutions of the form

$$v_M(P) = \sum_{j=1}^{M} a_k G(P, Q_j), \qquad P = (x, y) \in \Omega, \tag{5}$$

where $G(P,Q)$ is the fundamental solution of the operator L and $\{Q_j\}_1^M = \{(x_j, y_j)\}_1^M$ are M distinct points in the exterior of Ω. Usually v_M would not satisfy the boundary conditions for the given problem. Then we can choose M points $\{P_j\}_1^M$ on $\partial\Omega$ and force the boundary conditions at these collocation points.

For the Poisson operator $L = \Delta \equiv (\partial^2/\partial x^2) + (\partial^2/\partial y^2)$, the fundamental solution $G(P, Q) = (1/2\pi) \ln\|P - Q\|$. For completeness [28], it is more appropriate to add a constant C in Eq. (5) giving

$$v_M(P) = \sum_{j=1}^{M} a_j G(P, Q_j) + C, \qquad P = (x, y) \in \Omega,$$

in which case we need $M + 1$ collocation points $\{P_j\}_1^{M+1}$ on the physical boundary $\partial\Omega$ and let

$$v_M(P_i) = g(P_i) - \hat{u}_p(P_i), \qquad 1 \le i \le M + 1.$$

Hence we end up with solving the $M + 1$ system

$$\sum_{j=1}^{M} a_j G(P_i, Q_j) + C = g(P_i) - \hat{u}_p(P_i), \qquad 1 \le i \le M + 1,$$

for the unknown coefficients $\{a_j\}_1^M \cup \{C\}$.

3.3. The RBF-MFS

Instead of first approximating the right-hand side function of the equation and then find the approximate particular solution by analytical method, we can find the approximate particular solution directly by collocation method, i.e. by requiring the approximate particular solution

$$u_p(x, y) = \sum_{j=1}^{N} u_j \varphi_j(x, y), \tag{6}$$

to satisfy the underlying equation $Lu = f$ at the collocation points

$$\sum_{j=1}^{N} (L\varphi_j)(x_i, y_i) u_j = f(x_i, y_i), \qquad i = 1, 2, \dots, N. \tag{7}$$

Hence we end up with solving a $N \times N$ linear system with coefficient matrix $\mathbf{A} = [(L\varphi_j)(x_i, y_i)]$ for the unknowns $\{u_j\}_{j=1}^N$. Here N is the total number of collocation points.

Note that this technique was first proposed by Golberg in 1995 [25, p. 102] and was restated in the book of Golberg and Chen [16, p. 323]. Among many practioners in the BEM community, Chen and Tanaka [26] used multiquadric RBF $\varphi(r) = (r^2 + c^2)^{3/2}$ and Kögl and Gaul [27] used RBF $\varphi(r) = r^2 + r^3$ in their applications. But such applicability has never been justified mathematically before. Below we show that for the Poisson problem, the coefficient matrix resulting from our new DRM is guaranteed to be nonsingular for both Hardy's MQ and the cubic RBF.

Theorem 3.1. *For the Poisson operator $L = \Delta$, and the Hardy's MQ $\varphi(r) = \sqrt{r^2 + c^2}$ with arbitrary distinct N collocations points, the matrix $\mathbf{A} = [(L\varphi_j)(x_i, y_i)] = [(r_{ij}^2 + c^2)^{-1/2} + c^2(r_{i,j}^2 + c^2)^{-3/2}]$ is nonsingular for any shape parameter $c > 0$, where $r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$.*

Proof. For each collocation point (x_j,y_j), we denote

$$\varphi_j(x, y) = \sqrt{(x - x_j)^2 + (y - y_j)^2 + c^2} = \sqrt{r_j^2 + c^2},$$

$$r_j = \sqrt{(x - x_j)^2 + (y - y_j)^2}.$$

Thus, we have

$$\frac{\partial\varphi_j}{\partial x} = \frac{x - x_j}{\sqrt{r_j^2 + c^2}}, \qquad \frac{\partial\varphi_j}{\partial y} = \frac{y - y_j}{\sqrt{r_j^2 + c^2}},$$

$$\frac{\partial^2\varphi_j}{\partial x^2} = \frac{(y - y_j)^2 + c^2}{(r_j^2 + c^2)^{3/2}}, \qquad \frac{\partial^2\varphi_j}{\partial y^2} = \frac{(x - x_j)^2 + c^2}{(r_j^2 + c^2)^{3/2}}.$$

Therefore, we have

$$\mathbf{A} = [(r_{i,j}^2 + c^2)^{-1/2} + c^2(r_{i,j}^2 + c^2)^{-3/2}],$$

from which we see that $\mathbf{A}$ is a sum of two standard inverse MQ matries, by the fact that the inverse MQ are strictly positive definite function (see [16, p. 321,28, p. 121,29, p. 19]), we know that $\mathbf{A}$ is positive definite, which completes the proof.

Table 1
Comparisons between our RBF-MFS and Kansa's method on 10×10 mesh

RBFs	Kansa's method		RBF-MFS	
	Maximun relative error	Condition number	Maximum relative error	Condition number
$(r^2+c^2)^{1/2}$, $c=0.2$	1.070405×10^{-1}	3.3974×10^4	6.578783×10^{-1}	3.5403×10^3
$(r^2+c^2)^{1/2}$, $c=0.8$	5.745354×10^{-3}	3.4017×10^{12}	4.478028×10^{-2}	2.4183×10^{10}
$(r^2+c^2)^{1/2}$, $c=1.8$	2.144811×10^{-3}	1.0118×10^{18}	2.405268×10^{-3}	3.4017×10^{12}
r^3	5.551643×10^{-2}	1.2717×10^5	3.233604×10^{-1}	1.6709×10^3
r^5	4.058249×10^{-2}	2.6334×10^6	5.916529×10^{-2}	3.1743×10^5
r^7	3.705795×10^{-2}	2.8189×10^7	1.022251×10^{-2}	2.3759×10^7

□

Theorem 3.2. *For the Poisson operator $L = \Delta$, and the cubic basis function $\varphi(r) = r^3$ with arbitrary distinct N collocations points, the matrix $\mathbf{A} = [(L\varphi_j)(x_i, y_i)] = [9r_{ij}]$ is nonsingular, where $r_{ij} = \sqrt{(x_i-x_j)^2 + (y_i-y_j)^2}$.*

Proof. This follows directly from a result of Powell [28, p. 124] about the nonsingularity of interpolation matrix for RBF $\varphi(r) = r$.

□

Remark. *Theorems 3.1 and 3.2 hold true in 3-D by the same proofs as in 2-D, i.e. the matries $\mathbf{A} = [2(r_{ij}^2 + c^2)^{-1/2} + c^2(r_{i,j}^2 + c^2)^{-3/2}]$ (for $\varphi(r) = \sqrt{r^2+c^2}$) and $\mathbf{A} = [12r_{ij}]$ (for $\varphi(r) = r^3$) are nonsingular for distinct collocation points, where*

$$r_{ij} = \sqrt{(x_i-x_j)^2 + (y_i-y_j)^2 + (z_i-z_j)^2}.$$

Though theoretical proof of the nonsingularity of $\mathbf{A}$ for other RBFs is unachievable at present, our numerical tests on the uniformly distributed points showed the nonsingularity of $\mathbf{A}$ for thin plate splines $\varphi(r) = r^{2k} \ln r$, $k = 2, 3, \ldots$, in which case $\mathbf{A} = [(2k)^2 r^{2k-2} \ln r + 4kr^{2k-2}]$, Gaussian $\varphi(r) = \mathrm{e}^{-\beta r^2}$, in which case $\mathbf{A} = [(-4\beta + 4\beta^2 r_{i,j}^2)\, \mathrm{e}^{-\beta r_{i,j}^2}]$, and high order splines $\varphi(r) = r^{2k+1}$, $k = 2, 3, \ldots$, in which case $\mathbf{A} = [(2k+1)^2 r_{i,j}^{2k-1}]$. Some numerical results can be found in Table 2 below.

Table 2
The improved results for RBF-MFS by extending the 10×10 mesh by two more points in each direction

RBFs	RBF-MFS	
	Maximum relative error	Condition number
$(r^2+c^2)^{1/2}$, $c=0.2$	4.893924×10^{-2}	5.2490×10^3
$(r^2+c^2)^{1/2}$, $c=0.8$	1.326307×10^{-2}	8.5040×10^{13}
$(r^2+c^2)^{1/2}$, $c=1.8$	1.64008×10^{-2}	1.1586×10^{19}
r^3	4.548124×10^{-2}	4.2688×10^3
r^5	1.615172×10^{-2}	1.5393×10^6
r^7	2.181657×10^{-3}	2.2108×10^8
$r^4 \log r$	5.400945×10^{-2}	3.8984×10^4
$\mathrm{e}^{-\beta r^2}$, $\beta = 5$	3.268207×10^{-2}	4.0413×10^{17}

3.4. Numerical results for RBF-MFS

Here we solved the 2-D Poisson problem

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x,y), \qquad (x,y) \in \Omega, \ \ u|_{\partial\Omega} = g(x,y)$$

in the domain $\Omega = [0,1] \times [0,1]$, which is discretized by a 10×10 uniform grid. The function $f(x,y) = 13 \exp(-2x + 3y)$ and Dirichlet boundary function $g(x,y)$ were chosen such that the exact solution is

$$u(x,y) = \exp(-2x + 3y).$$

This problem was considered previously by Kansa [1, p. 159], where he obtained the maximum norm error 0.4480 with only 10 boundary points and 20 interior points.

The results obtained by Kansa's method and RBF-MFS are presented in Table 1. In RBF-MFS we used 20 uniformly distributed source points on the fictitious boundary of a circle with radius 5.

From Table 1, we see that RBF-MFS can achieve comparable results as Kansa's method, direct comparison with the classic MFS-DRM is not pursued here because we have recently found that the classic MFS-DRM and Kansa's method have achieved similar accuracy [33].

After careful checking the error at each collocation point, we found that we can improve the results by adding some collocation points outside the domain Ω so that we can obtain better approximation for the particular solution at the boundary points of Ω. We rerun the above problem by extending two more points outside the domain in each direction, the accuracy does improve a lot, as shown in Table 2.

4. Conclusions

The RBF-MFS is revisited, and is theorectically proved solvable and numerically comparable with Kansa's method. Note that RBF-MFS avoids the perplexity about the solvability of Kansa's method [11] and the complexity of finding the analytical particular solution in the classic MFS-DRM [16]. The generalization of this method to other problems is currently under investigation.

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