Preconditioning for Radial Basis Functions with Domain Decomposition Methods

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Abstract: *Over the last decade or so, researchers have investigated the use of RBFs in the numerical solutions of ordinary (ODEs) and partial differential equations (PDEs). In general, when using RBFs to solve PDEs, the resulting matrices are full and severely ill-conditioned. Therefore, applications of RBF-PDE were once restricted to problems of moderate size solved with direct methods. We address this problem with a preconditioning technique based on approximate cardinal basis functions (ACBFs). We then couple the ACBF preconditioning technique with the domain decomposition method (DDM) which allows one to solve large-scale PDE problems in parallel.*

1 Background

A major class of preconditioners for the RBF interpolation problem is the null space method, see [1, 2]. Such a method relies on the fact that most popular RBFs are strictly conditionally positive definite of order m (SCPDm).The resulting preconditioners are of size $(N-m)$-by-$(N-m)$. The preconditioned systems are positive definite and are commonly solved by the conjugate gradient method. Bozzini, Lenarduzzi, and Schaback [3] use increasing annihilation orders of B-splines to improve the decay rates thereby improving the convergence rates of multiquadrics and polyharmonic splines. However, this class of preconditioner cannot be extended to the application of PDEs since the resulting RBF-PDE coefficient matrix does not enjoy the SCPD property.

Another important preconditioning technique is the approximate cardinal basis function (ACBF) approach. In this approach, the preconditioner has the same dimension as the original matrix. At a point x_i, an ACBF is merely a linear combination of the neighboring RBFs. Beatson et al. [4] lower the computational cost of solving the RBF interpolation

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problem to $O(N \log N)$ operations. Faul improved the efficiency by combining the above ideas with Jacobi iteration and avoiding the unnecessary evaluation of residuals, see [5, 6]. Interested readers can find more studies of cardinal functions of MQ by Buhmann and Micchelli [7], and Baxter [8].

Consider a PDE of the form,

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

The unknown PDE solution u is approximated by RBFs,

$$
u = \sum_{k=1}^{N} \alpha_k \phi(x - x_k).
\tag{2}
$$

To solve for the N unknown coefficients $\alpha = [\alpha_1, \ldots, \alpha_N]^T$, N linearly independent equations are needed. These equations can be obtained by choosing N distinct collocation points $X = \{x_1, \ldots, x_N\}$ on both $\Omega \setminus \partial\Omega$ and $\partial\Omega$. We assume the points (centers) are arranged in such a way that the first N_I points and the last N_B points are in $\Omega \setminus \partial\Omega$ and $\partial\Omega$, respectively. The centers x_k used in (2) are often chosen as collocation points. Other strategies of choosing X were studied by Fornberg et al. [9]. Ensuring that $U(x)$ satisfies (1) at the collocation points results in a good approximation of the solution u. The equations are

$$
\begin{aligned}
\sum_{k=1}^{N} \alpha_k \mathcal{L}\phi(x_i - x_k) &= f(x_i) \quad \text{for } x_i \subset X \cap (\Omega \setminus \partial\Omega), \\
\sum_{k=1}^{N} \alpha_k \mathcal{B}\phi(x_i - x_k) &= g(x_i) \quad \text{for } x_i \subset X \cap \partial\Omega.
\end{aligned}
\tag{3}
$$

Rewriting (3) in matrix form, we have

$$
A\alpha = b, \quad \text{where } A = \begin{bmatrix} A_{\mathcal{L}} \\ A_{\mathcal{B}} \end{bmatrix}, \; b = \begin{bmatrix} f(x_i) \\ g(x_i) \end{bmatrix},
\tag{4}
$$

and

$$
\begin{aligned}
(A_{\mathcal{L}})_{ik} &= \mathcal{L}\phi(x_i - x_k), \quad x_i \subset (\Omega \setminus \partial\Omega), \quad x_k \in X, \\
(A_{\mathcal{B}})_{ik} &= \mathcal{B}\phi(x_i - x_k), \quad x_i \subset \partial\Omega, \qquad\quad x_k \in X.
\end{aligned}
\tag{5}
$$

This method is often named the asymmetric collocation method. The symmetric collocation approach can be found in [10]. The matrix given by (4) and (5) is generally non-symmetric and full; this system of equations is known to be very ill-conditioned when N or c becomes large.

We present a new preconditioner designed to work on the asymmetric collocation method for various RBF-PDE applications. This preconditioner is sufficiently general that it may be applied to elliptic, hyperbolic or parabolic PDEs in which RBFs are used as the spatial approximation scheme. Furthermore, the preconditioning technique is coupled with the domain decomposition method.

2 Our results

We have developed an effective preconditioner scheme for the asymmetric collocation scheme in which radial basis functions (RBFs) are used to solve partial differential equations (PDEs) problems. This method works well for elliptic, hyperbolic and parabolic PDEs and for the volume integral PDE formulation [11].

An ideal approximate cardinal basis function (ACBF) is equivalent to a delta function $\delta(x_i)$ that is one at it center x_i and zero everywhere else. We start from the coefficient matrix A that is constructed from the PDE boundary condition and interior operators acting upon the RBFs. For each center x_i, we select a set containing special points and local neighboring centers of size $m \ll N$. The inclusion of special points in this subset that ensures each ACBF is more distinct in shape.

We find the set of weights w_i at each center by solving each least-squares problem to construct the global preconditioner W. The set of least-squares problems is solved using either a local normal equation approach (L-NE), a local QR factorization (L-QR), or a local singular value decomposition (L-SVD) method.

The preconditioner W is constructed from the sets of weights w_i that transforms the elements of the RBF-PDE coefficient matrix A into ACBFs. The preconditioner W that acts as an approximation to A^{-1} clusters the real part of the complex eigenvalues of WA about 1 permitting the solution of the RBF expansion coefficients to be solved by the very efficient GMRES iteration scheme. With the set of expansion coefficients determined, we reconstruct the numerical solution u over the domain of interest.

Our intent is to be able to obtain max and mean root square errors with our preconditioning scheme that are less than or equal to the same errors obtained by global Gaussian elimination, but requiring far fewer flops. In its present form, our preconditioner represents a major breakthrough in the computational efficiency of the RBF-PDE method. However, we make the caveat that this computational efficiency holds as long as safe values of the shape parameter are used to prevent severe ill-conditioning in both the global RBF-PDE coefficient matrix A and the normal equation matrices that are used to construct the preconditioner W.

The numerical solutions obtained from GMRES iteration on an elliptic PDE test problem found in [12] are reported. We tested the ACBF method for various size problems and values of the MQ shape parameter $c(N)$ for regularly spaced and scattered center distributions. We found that the shape parameter plays a very important role.

The other attractive possibility of using larger values of c and/or N is to combine our preconditioner with the domain decomposition method (DDM), [14, 15, 16, 17, 18]. DDM splits Ω into K overlapping or nonoverlapping subdomains, each of which contains $N_k \ll N$ centers. The smaller dimension coefficient matrices are orders of magnitude better conditioned than the corresponding global coefficient matrix. Smith, Bjørstad, and Gropp [?] present a nice overview of the techniques used for overlapping and nonoverlapping methods that are applicable in the efficient solution methods for PDE problems on parallel machines that are readily transferable to RBF-PDE methods.

With DDM, both the original and preconditioned systems on the subdomains are better conditioned when we are dealing with $N_k < N$ centers instead of N centers. Furthermore, combining our preconditioning technique with DDM will permit the use of a larger shape parameter by increasing the m/N ratio on each subdomain keeping the number of flops within an economical limit.

We acknowledge that our preconditioning scheme requires more development, but it still performs very efficiently with the caveat that we restrict the condition number of global coefficient matrix A by using safe values of $c \sim h_{\min}$. Then the GMRES iteration scheme converges within tens of iterations. The current preconditioner is two to three orders more efficient than global Gaussian elimination methods, and GMRES is N times more efficient than G-GE as N increases.

For cases where the condition number of A is about 10^{10} to 10^{13} and $1089 \leq N \leq 1681$, our preconditioning scheme only requires approximately 25% of the flops of the G-GE method. For highly ill-conditioned problems, the preconditioned GRMES is able to converge for A having a condition number as high as 10^{15}, but GMRES now requires about 80% of the number of flops compared to G-GE.

In the next investigation, we will combine overlapping domain decomposition methods (DDM) with the least-squares ACBF method. We obtained considerable efficiency in our scheme by using the fast matrix-vector multiplication scheme of [4, 19]. However, we intend to obtain even better efficiencies when we implement the fast multipole expansion method of Beatson and Newsam[20] and combine our ACBF with domain decomposition similar to work of Beatson, Light, and Billings [14]. Another promising approach would be to combine the ideas presented by Bozzini et al. [3]; by constraining the ACBFs to have higher order vanishing moments, the ACBFs decay very rapidly obviating the need to include the majority of the column elements of A. Such a combination is especially attractive for large-scale problems of engineering interest for the following reasons:

- No labor intensive mesh generation is required.

- The RBF-PDE collocation method is very simple to implement.

- The rate of convergence of MQ-RBF methods is exponential compared to the linear or quadratic convergence rates of the traditional methods.

- We will optimize the flop rates for the GMRES method using similar fast methods as Beatson and co-workers.

- As the number of subdomain increase, the partitioned matrix A_k associated with each subdomain becomes better conditioned, permitting larger c values with the accompanying faster convergence and coarser discretization requirements.

- With the work load distributed among many processors, the turn-around time to finish a run diminishes, permitting a larger number of parametric studies to be completed.

This DDM-ACBF approach can be very relevant when combined with Fornberg's method. We intend to provide persons who are interested in using asymmetric RBF-PDE methods various options to solve their problems. It is hoped that our work will dispel the perception that only finite difference, element, and volume methods are computationally efficient methods to solve PDE problems in view of their slow convergence rates.

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