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An improved radial basis-pseudospectral method with hybrid Gaussian-cubic kernels

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ABSTRACT

While pseudospectral (PS) methods can feature very high accuracy, they tend to be severely limited in terms of geometric flexibility. Application of global radial basis functions overcomes this, however at the expense of problematic conditioning (1) in their most accurate flat basis function regime, and (2) when problem sizes are scaled up to become of practical interest. The present study considers a strategy to improve on these two issues by means of using hybrid radial basis functions that combine cubic splines with Gaussian kernels. The parameters, controlling Gaussian and cubic kernels in the hybrid RBF, are selected using global particle swarm optimization. The proposed approach has been tested with radial basis-pseudospectral method for numerical approximation of Poisson, Helmholtz, and Transport equation. It was observed that the proposed approach significantly reduces the ill-conditioning problem in the RBF-PS method, at the same time, it preserves the stability and accuracy for very small shape parameters. The eigenvalue spectra of the coefficient matrices in the improved algorithm were found to be stable even at large degrees of freedom, which mimic those obtained in pseudospectral approach. Also, numerical experiments suggest that the hybrid kernel performs significantly better than both pure Gaussian and pure cubic kernels.

1. Introduction

Pseudospectral (PS) methods are highly accurate and higher-order numerical methods, which use polynomials as basis functions. In two or higher dimensions, PS method tend to be limited in terms of geometric flexibility [1]. A typical variant of PS methods is Chebyshev pseudospectral method (CHEB-PS), which uses Chebyshev polynomials as basis functions. In order to make the PS method geometrically flexible, Fasshauer [2] proposed the application of infinitely smooth radial basis functions (RBFs) in pseudospectral formulation and interpreted the combined approach as meshless radial basis-pseudospectral (RBF-PS) method. Gaussian RBF is one such infinitely smooth RBF, which results in a positive definite system ensuring uniqueness in the interpolation. It is often found in the application of smooth RBFs that scaling the radial kernel by reducing the shape parameter to a smaller value, i.e., making it “flat” reduces the error in the approximation, as the “flat” limit of infinitely smooth RBF converges to a polynomial interpolant [3,4]. Larsson and Fornberg [5] have shown that it is possible to get even more accurate results with Gaussian RBF in the “flat” range, *i.e*, just before it converges to polynomial interpolants. Although global RBF methods are relatively costly because of the full and dense matrices arising in the linear system, their accuracy and convergence makes them desirable, especially for problems in solid mechanics. In recent years, RBF-PS method has been effectively applied to computational mechanics [6–8], nonlinear equations [9], and thermal convection in 3D spherical shells [10], etc. Application of an infinitely smooth RBF in pseudospectral mode, however, brings an inherent limitation, as the global approximation of RBFs gets severely ill-conditioned at higher degrees of freedom as well as at low shape parameters. Such limitations constraint the well-posedness of the RBF-PS algorithm only to few nodes in the domain with relatively large shape parameter range. Typical quantification of such limitations can be found in [2], where the RBF-PS algorithm was found to be well-posed upto 24×24 nodes for 2D Helmholtz's equation and 18 nodes for 1D transport equation.

To deal with the ill-conditioning in RBF interpolation, Kansa and Hon [11] performed numerical tests using various tools, viz., block partitioning or LU decomposition, matrix preconditioners, variable shape parameters, multizone methods, and node adaptivity. Other major contributions to deal with the mentioned problem are: a direct

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solution approach [12], accelerated iterated approximate moving least squares [13], random variable shape parameters [14], Contour-Padé and RBF-QR algorithms [15], series expansion [16], and regularized symmetric positive definite matrix factorization [17], RBF-GA [18], Hilbert-Schmidt SVD [19], Weighted SVD [20], use of Laurent series of the inverse of the RBF interpolation matrix [21], and RBF-RA [22], *etc*. An alternative approach is radial basis finite difference (RBF-FD) method, which is a local version of RBF-PS method [23–26]. The only significant difference between RBF-PS and RBF-FD implementation is that instead of using all the nodes, later uses only few neighbour nodes for construction of differential matrices.

Recently, Mishra et al. [27] proposed novel radial basis functions by hybridizing Gaussian and cubic kernels, which could significantly reduce the ill-conditioning problem in scattered data interpolation. This hybrid kernel utilizes optimal proportion of the Gaussian and cubic kernel, which correspond to the defined optimization criterion. In this paper, we propose a well-conditioned radial basis-pseudospectral scheme for numerical approximation of PDEs, by incorporating hybrid Gaussian-cubic kernels as basis functions. We establish both the convergence and stability of this improved scheme, through several numerical examples including numerical approximation of time-independent and time-dependent PDEs. Hereafter, in this work, we will call this improved approach as hybrid radial basis function-pseudospectral approach (HRBF-PS).

Rest of the paper is structured as follows. We introduce the hybrid RBF in Section 2, and the global particle swarm optimization algorithm for selecting the parameters of this hybrid RBF in Section 3. Construction of differentiation matrices, and the RBF-PS scheme for numerical solution of PDEs have been explained in Section 4. Finally we perform numerical tests by solving Poisson, Helmholtz, and transport equations using the improved RBF-PS method and exhibit the improvements, observed due to hybrid RBF over Gaussian and Cubic RBFs, in Section 5, followed by the conclusion. In Appendix A, we explain the particle swarm optimization algorithm and its application in the contexts of numerical solution of PDEs with meshless methods.

2. Hybrid Gaussian-cubic RBF

Radial basis functions were proposed by Hardy [28] for fitting topography on irregular surfaces using linear combination of a single symmetric basis functions, which was later found to have better convergence than many available approaches for interpolation [29]. Some commonly used RBFs have been listed in Table 1. First application of RBFs for numerical solution of differential equations was proposed by Edward Kansa in 1990 [30]. Since RBFs do not require to be interpolated on regular tensor grids, Kansa's method did not require“mesh”, therefore, it was termed as a meshless method. Infinitely smooth RBFs like Gaussian have been proven to provide invertible system matrix in such meshless methods. However, for small shape parameters, as well as large number of nodes in the domain, Gaussian RBF leads to solving an ill-conditioned system of equations. Cubic RBFs on the other hand, are finitely smooth radial basis functions, which, unlike Gaussian RBF, do not have any shape parameter. However, use of cubic RBF for shape function interpolation in meshless methods involves the risk of getting a singular system, for certain node arrangements. Recently, a hybrid RBF [27], by combining Gaussian and the cubic kernels, has been proposed which could utilize certain features of both the RBFs depending on the problem type under consideration, as given by

$$\phi(r) = \alpha e^{-(\epsilon r)^2} + \beta r^3, \tag{1}$$

where, ϵ is the shape parameter of the radial basis function, which is a relatively new notation for the same. One advantage of using this new conventions is that all the RBFs depend on the shape parameter in a similar manner. It should be noted that there is another parallel convention for the shape parameter, which is commonly represented as ‘*c*’ [31]. The conversion from old to new convention can be done by setting $c^2 = 1/\epsilon^2$ [32]. The weight coefficients α and β control the contribution of Gaussian and cubic kernel in the proposed hybridization depending upon the problem type.

Table 1
Some frequently used radial basis functions (radial kernels) and their mathematical expressions.

Kernel	Mathematical expression
Multiquadratic (MQ)	$(1+(\epsilon r)^2)^{1/2}$
Inverse multiquadratic (IMQ)	$(1+(\epsilon r)^2)^{-1/2}$
Gaussian (GA)	$e^{-(\epsilon r)^2}$
Polyharmonic Spline (PHS)	$\begin{cases} r^m ln(r) & m=2,4,6,\ldots \\ r^m & m=1,3,5,\ldots \end{cases}$
Wendland's (Compact Support)	$(1-\epsilon r)_+^4(4\epsilon r+1)$

3. Parameter optimization

Since the shape parameter affects both the accuracy and stability of algorithms involving RBFs, finding its optimal value has been a critical issue in radial basis interpolation and its application in meshless methods [33–35]. The hybrid kernel, presented in this study, contains three parameters, i.e., ϵ, α, and β, an optimal combination of which will ensure the optimum convergence and stability of the associated algorithm. Particle swarm optimization (PSO) is a frequently used algorithm to decide the shape parameter in RBF network and its application in machine learning algorithm [36,37], however in context of numerical approximation of PDEs with meshless methods, it is generally decided with ad-hoc methods like solving the problem with various values of the shape parameter and visualizing the root mean square (RMS) error against it. This approach works only if the exact solution of the problem is known, which in practical cases, is often unknown. For such cases, in the context of scattered data interpolation, Rippa [38] proposed a statistical approach using leave-one-out-cross-validation (LOOCV), which later got generalized for numerical solution of PDEs, by Fasshauer [39]. Here we use a global particle swarm optimization algorithm, to decide the optimal values of the parameters of the hybrid kernel. We test two different objective functions: (1) RMS error, when the exact solution is known and (2) LOOCV criterion, when the exact solution is not known. Algorithm (1), explains the process of computing the objective function using LOOCV. Here c_k is the *kth* coefficient for the interpolant on “full data” set and $\mathbf{A}_{kk}^{-1}$ is the k^{th} diagonal element in the inverse of the interpolation matrix for “full data”. A detailed discussion about the application of particle swarm optimization in this context has been given in Appendix A.

Algorithm 1. LOOCV for computing the objective function for parameter optimization. This algorithm uses the interpolation matrix, which is computed to construct various differentiation matrices in RBF-PS.

1: Fix a set of parameters $[\epsilon, \alpha, \beta]$
2: **for** all the N collocation points, i.e.,k=1,...,N **do**
3: **if** using Rippa's simplified approach [38] **then**
4: Compute the error vector e_k as

$$e_k = \frac{c_k}{\mathbf{A}_{kk}^{-1}}. \tag{2}$$

5: **else**
6: Compute the interpolant by excluding the k^{th} point as