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A modification on strictly positive definite RBF-DQ method based on matrix decomposition

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ABSTRACT

The infinitely smooth RBF methods are theoretically spectrally accurate for applying on scattered data interpolation, and also partial differential equations, but the interpolation matrices of them are extremely ill-conditioned especially for strictly positive definite ones. Therefore, an efficient technique to recover this problem is too important. In this article, a general matrix decomposition method for strictly positive definite RBFs interpolation matrix has been investigated. In the current decomposition the RBFs interpolation matrix is obtained as multiplication of some well-conditioned matrices. This decomposition has been applied to RBF-DQ method and its results more accurate weight coefficients when we involve solving PDEs.

1. Introduction

Scattered data interpolation, especially in irregular domains or higher dimensional geometry, is an important problem in science and engineering. Accordingly conventional methods such as polynomial and spline interpolations have been employed for a wide range of science and engineering problems, but using these functions are not so efficient in higher-dimensional or scattered nodes in irregular domains. In practice, these bases directly related to the arrangement of the nodes and may not be used for any scattered sets. Consequently radial basis function (RBF) interpolation is an alternative for such a purpose.

RBF was first studied by Roland Hardy in 1968. This method allows scattered data to be easily used in computations. Franke [1] supervised a deeper study in the area of interpolation methods, and the consequences were RBFs interpolations, a very accurate technique, comparing with other available techniques. An advantage of the theory of RBFs interpolation was and also is, that it prepares a smooth interpolation of some discrete data. Kansa [2] first, used RBFs to solve differential equations (DEs) as an approximation to the solution. However, in recent years RBFs have been extensively researched and applied in a wider range of analysis. Variety problems have been solved by RBFs [3–7].

Some more applicable RBFs, are listed in Table 1 where $r = \| \mathbf{x} - \mathbf{x_i} \|_2$ and ϵ is free positive shape parameter, where should be valued by user or perhaps specifying some values from the problem lead to convergence and stability. Ranges from too large to too small shape parameter ϵ reshape the GA from flat to peaked. Despite many researchers work on finding an algorithm to predict some optimum values for shape number, it is still under investigation and it seems that, this phenomena so far is an open problem [8–10]. In Inverse Quadratic, Inverse Multiquadric, Generalized Inverse Multiquadrics (GIMQ), Hyperbolic Secant (sech), Gaussian (GA), Inverse-Quadratic Gaussian (IQG) (defined by Boyd and McCauley [11]) and Matérn functions, the interpolation matrices are positive definite, and for Multiquadrics (MQ), it has only one positive eigenvalue [12]. The infinitely smooth RBF methods are theoretically spectrally accurate for applying on scattered data interpolation, and also partial differential equations. In all these cases the interpolation coefficient matrices are extremely ill-conditioned especially for strictly positive definite RBFs. The condition number of the matrix exponentially grows up as the minimum separation distance due to increasing the number of nodes decreases, and also as the shape parameter decreases, and these reasons yield to increase in computational error of solving the system even by applying the SPD system solvers such as Cholesky and the square root free Cholesky factorization [13]. For smooth functions, a reasonable accuracy for a given number of nodes, may be obtained provided the shape parameter is small [14], conversely the instability associated small shape parameters lead to an unreliable approximation. Fornberg and Wright [15,16] developed an algorithm named Contour-Padé to gain the stability for small shape parameter and therefore refuses the uncertainty principle which Schaback [17] described. This algorithm is suitable for the case of flat RBFs

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Table 1
Some radial basis functions (RBFs).

Multiquadric (MQ)	$\sqrt{1+(\epsilon r)^2}$	Inverse Multiquadric (IMQ)	$1/\sqrt{1+(\epsilon r)^2}$
Gaussian (GA)	$\exp(-(\epsilon r)^2)$	Inverse Quadratic (IQ)	$1/(1+(\epsilon r)^2)$
Conical Splines (CS)	r^{2k+1}	Third Power of Multiquadric	$(1+(\epsilon r)^2)^{3/2}$
Hyperbolic Secant	$\mathrm{sech}(\epsilon r)$	Thin Plate (polyharmonic) Splines	$(-1)^{k+1} r^{2k}\log r$

nevertheless needs some restrictions on the number of nodes. Also Forenberg and Piret [18] introduced the RBF-QR algorithm which is computationally stable for flat RBFs interpolation, and is easier to implement rather than Contour-Padé and also it can be implemented in a large number of nodes. Also, this algorithm has been generalized for node distributions in 2-d or 3-d [19,14]. Also Fasshauer and Mccourt [20] have provided a new way to compute and evaluate Gaussian RBF interpolation with small values of shape parameter which is motivated by the fundamental ideas of RBF-QR in a simple way.

The extension of precision floating point arithmetic, improve the accuracy of RBF methods [4,13]. Also Sarra recently has proposed a regularization scheme to improve the accuracy of SPD matrix factorizations created from positive definite RBFs interpolation, and also prevent the failure of the Cholesky factorization [21].

In the present work, a general decomposition for strictly positive definite RBFs interpolation matrix has been constructed by the fundamental ideas of the technique which is called the method of diagonal increments (MDI) [22,23]. This decomposition converts the interpolation matrix to the product of some matrices which are well-conditioned.

2. Radial basis functions

Let ϕ: $[0, \infty) \to [0, \infty)$ be a continuous function. A radial basis function on $\mathbb{R}^d$ (for some positive integer d) is a function of the form $\phi(\| \mathbf{x}-\mathbf{x_0} \|_2)$, $\mathbf{x} \in \mathbb{R}^d$, and $\mathbf{x}_0$ is any fixed point in $\mathbb{R}^d$, also $\|.\|_2$ denotes the Euclidean norm. For any arbitrary collection of N nodes $\{\mathbf{x}_i\}_{i=1}^N$ in $\mathbb{R}^d$ the function

$$s(\mathbf{x}) = \sum_{j=1}^{N} a_j \phi(\| \mathbf{x}-\mathbf{x}_j \|_2), \quad a_j \in \mathbb{R},$$

is called a radial function as well [24], obviously a radial function is invariant under all rotations leaving the origin fixed.

2.1. RBFs interpolation

Let f be a real function defined on a domain in $\mathbb{R}^d$. An RBFs approximation f_N to the function f subordinate to N points $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$ belonging to its domain may define as follows:

$$f(\mathbf{x}) \approx f_N(\mathbf{x}) = \sum_{j=1}^{N} a_j \phi_j(\mathbf{x}), \tag{1}$$

where $\phi_j(\mathbf{x}) = \phi(\| \mathbf{x}-\mathbf{x}_j \|_2)$, $\mathbf{x}$ is the input vector, and a_j, $j = 1, 2, \ldots, N$ are unknown numbers, to be determined by N nodes $\{\mathbf{x}_j\}_{j=1}^N$ through the linear system

$$f_i := f(\mathbf{x}_i) = \sum_{j=1}^{N} a_j \phi_j(\mathbf{x}_i), \quad i = 1, 2, \ldots, N. \tag{2}$$

Taking $\mathbf{f} = [f_1, f_2, \ldots, f_N]^T$ and $\mathbf{a} = [a_1, a_2, \ldots, a_N]^T$ give the following matrix form

$$\mathbf{\Phi a} = \mathbf{f}, \tag{3}$$

where

$$\mathbf{\Phi} = \begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \ldots & \phi_N(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \ldots & \phi_N(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{x}_N) & \phi_2(\mathbf{x}_N) & \ldots & \phi_N(\mathbf{x}_N) \end{bmatrix}. \tag{4}$$

The matrix $\mathbf{\Phi}$ is symmetric because of $\phi_i(\mathbf{x}_j) = \phi_j(\mathbf{x}_i)$. It's also a nonsingular matrix [12], and hence there exists a unique interpolant form for the function f. This approximation can be applied for all infinitely smooth RBFs that are listed in Table 1 and for any collection of nodes. Obviously the linear system (3) is ill-conditioned for any infinitely smooth RBFs, therefore for big N, the linear system (3) faces with a large computational error with majority linear system solvers. The solvability of the linear system (3) is directly related to $\kappa(\mathbf{\Phi})$ the condition number of the matrix $\mathbf{\Phi}$,

$$\kappa(\mathbf{\Phi}) = \| \mathbf{\Phi} \|_2 \| \mathbf{\Phi}^{-1} \|_2 = \frac{\sigma_{max}}{\sigma_{min}}, \tag{5}$$

where σ_{max} and σ_{min} are the largest and smallest singular values of $\mathbf{\Phi}$ respectively. In this work, we focus only on positive definite RBFs, so we give some basic definitions and properties of these type of functions.

Definition 1. A continuous complex function Φ defined on $\mathbb{R}^d$ is called *positive definite* on $\mathbb{R}^d$ if

$$\sum_{j=1}^{N} \sum_{k=1}^{N} c_j \bar{c}_k \Phi(\mathbf{x}_k - \mathbf{x}_j) \ge 0, \tag{6}$$

holds for any N pairwise distinct points $\mathbf{x}_j \in \mathbb{R}^d$, $j = 1, 2, \ldots, N$, and any N complex numbers c_j, $j = 1, 2, \ldots, N$. The function Φ is called *strictlypositivedefinite* on $\mathbb{R}^d$ if it is positive definite and the quadratic form (6) is equal to zero only for trivial c_j, $j = 1, \ldots, N$.

Definition 2. A continuous function ϕ: $[0, \infty) \to \mathbb{R}$ which is infinitely many times differentiable on $(0, \infty)$ and satisfying in the following properties

$$(-1)^l \phi^{(l)}(r) \ge 0, \quad \forall\, r > 0, \quad l = 0, 1, 2, \ldots,$$

is called *completelymonotone* on $[0, \infty)$. Schoenberg found a relation between positive definite radial functions and completely monotone function as follows.

Theorem 1. *A function ϕ is completely monotone on $[0, \infty)$ if and only if $\phi(\|\cdot\|_2^2)$ is positive definite on every $\mathbb{R}^d$* [25,27].

Theorem 1 is a criterion to check out which radial functions are strictly positive definite. Obviously we have the following results for strictly positive definite RBFs

$$\| \mathbf{\Phi} \|_2 = \lambda_{max}, \quad \| \mathbf{\Phi}^{-1} \|_2 = \frac{1}{\lambda_{min}}, \quad \kappa(\mathbf{\Phi}) = \frac{\lambda_{max}}{\lambda_{min}}, \tag{7}$$

where λ_{max} and λ_{min} are the largest and the smallest eigenvalues of $\mathbf{\Phi}$, respectively. Clearly for positive definite RBFs λ_{min} approaches to zero while the λ_{max} tends to ∞, as N increases and therefore the condition number rapidly increases accordingly. Suppose $\lambda_j > 0$, $j = 1, \ldots, N$ are all eigenvalues of the matrix $\mathbf{\Phi}$, and since all entries on diagonal of this matrix are equal to $\phi(0) = 1$, we deduce

$$\lambda_{max} < \sum_{j=1}^{N} \lambda_j = \mathrm{trace}(\mathbf{\Phi}) = N\phi(0) = N, \tag{8}$$

hence third part of (7) yields

$$\kappa(\mathbf{\Phi}) < \frac{N}{\lambda_{min}},$$

which guaranties an upper bound for $\kappa(\mathbf{\Phi})$ if λ_{min} is not less than the machine precision. There are some lower bounds for λ_{min} as follows.

$$\lambda_{min} \ge C_d(\sqrt{2}\epsilon)^{-d}\, \mathrm{e}^{-\frac{40.71 d^2}{(\epsilon q_X)^2}} q_X^{-d}, \quad \text{GA–RBF}, \tag{9}$$