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A stable method for the evaluation of Gaussian radial basis function solutions of interpolation and collocation problems

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ABSTRACT

Radial basis functions (RBFs) are a powerful tool for approximating the solution of high-dimensional problems. They are often referred to as a meshfree method and can be spectrally accurate. The best accuracy can often be achieved when the so-called shape parameter of the basis functions is small, which in turn tends to make the interpolation matrix increasingly ill-conditioned. To overcome such instability in the numerical method, which arises for even the most stable problems, one needs to stabilize the method. In this paper we present a new stable method for evaluating Gaussian radial basis function interpolants based on the eigenfunction expansion for Gaussian RBFs. This work enhances the ideas proposed in Fasshauer and McCourt (2012), by exploiting the properties of the orthogonal eigenfunctions and their zeros. We develop our approach in one and two-dimensional spaces, with the extension to higher dimensions proceeding analogously. In the univariate setting the orthogonality of the eigenfunctions and our special collocation locations give rise to easily computable cardinal basis functions. The accuracy, robustness and computational efficiency of the method are tested by numerically solving several interpolation and boundary value problems in one and two dimensions. High accuracy, simple implementation and low complexity for high-dimensional problems are the advantages of our approach. On the down side, our method is currently limited to the use of tensor products of unevenly spaced one-dimensional data locations.

1. Introduction

In the past three decades, radial basis functions (RBFs) have been used in many branches of science such as numerical analysis, statistics, geophysics, astrophysics, quantum mechanics, etc. So far, several books have been written on the theory and implementation of RBFs (see [1–5]). Radial basis functions are a powerful tool for interpolation and approximation of high-dimensional problems, and also for the solution of partial differential equations (PDEs) with scattered collocation points. One of the big advantages of using RBF is the spectral convergence rate that can be achieved when using infinitely smooth basis functions such as Gaussians. The best accuracy can often be achieved when the shape parameter in the basis function is small, i.e. when the RBF is near-flat. But as the shape parameter becomes small, the interpolant matrix becomes increasingly ill-conditioned. For many years, researchers mistakenly believed that the error and the condition number cannot both be kept small simultaneously. This is known as the uncertainty principle, see [6]. Today, however, we know that the uncertainty principle applies when one uses the direct or standard basis method to express the RBF interpolant.

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This insight has led to a growing number of stable approaches to overcome this problem. The first approach was the Contour-Padé approach derived by Fornberg and Wright [7]. The algorithm stably calculates the RBF approximant for small values of the shape parameter in any number of dimensions, but it is limited to a small number of collocation points. Another approach is the RBF-QR method which was introduced by Fornberg and Piret in 2007 for the case when the collocation points are distributed over the surface of a sphere [8]. The RBF-QR method for interpolation with Gaussian kernels was extended to more general domains in [9,10] using products of Chebyshev polynomials and spherical harmonics. A fundamental difference between various alternate (and potentially stable) basis approaches for kernel methods comes down to whether the kernel matrix K is formed and then operated upon to obtain a QR or SVD factorization such as [11,12], or whether a stable factorization of K is constructed by starting with a given series expansion of the kernel K, such as [13,9]. In [13], Fasshauer and McCourt developed a variant of the RBF-QR method by using an eigenfunction expansion of the Gaussian RBF. By considering the Gaussian as a special case of a positive definite kernel they established a connection between the RBF-QR algorithm and Mercer's theorem. McCourt [14] used this Gaussian eigenfunction approach to solve boundary value problems. In [11], an alternate stable basis derived via a weighted singular value decomposition of the kernel matrix was presented.

In this paper, we enhance the eigenfunction expansion approach for evaluating Gaussian RBF interpolants by taking advantage of the orthogonality of the eigenfunctions and collocating at their zeros. This allows us to construct a new stable factorization of the interpolation matrix K (without actually forming K and then decomposing it). Similar to the works [13,9], we employ series expansions to eliminate the destructive effect of a very small shape parameter, which is known to be one of the sources of ill-conditioning. We apply the method for interpolation of function values and collocation solution of boundary value problems in one and two space dimensions.

The rest of the paper is organized as follows. In the next section we will present some preliminary concepts about eigenfunction expansions. Our new stable method for Gaussian RBF interpolation is investigated in Section 3. The solution of boundary value problems using RBF-based collocation is investigated in Section 4 and finally some numerical results that illustrate the accuracy and efficiency of the proposed method are included in Section 5.

2. Eigenfunction expansion for Gaussian RBFs

Before discussing the eigenfunction expansion of Gaussian RBFs, we present a brief summary about Hermite polynomials. For each $n \in \mathbb{N}_0$, the function $H_n : \mathbb{R} \to \mathbb{R}$ defined by Rodrigues' formula

$$H_n(x) = (-1)^n \mathrm{e}^{x^2} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \mathrm{e}^{-x^2}, \tag{1}$$

is known as Hermite polynomial of degree n. These polynomials also satisfy the following recursion relation:

$$\begin{cases} H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), & n \geq 0, \\ H_{-1}(x) = 0, \qquad H_0(x) = 1. \end{cases}$$

The set $\{H_n : n \in \mathbb{N}_0\}$ is orthogonal with respect to the weight e^{-x^2}:

$$\int_{-\infty}^{\infty} \mathrm{e}^{-x^2} H_n(x) H_m(x) dx = 2^n n! \sqrt{\pi}\, \delta_{mn}.$$

In order to obtain an accurate approximate solution, it is better to normalize the Hermite polynomials. In this paper we use the normalized Hermite polynomials defined by $\widetilde{H}_n(x) = \frac{1}{\sqrt{2^n n!}} H_n(x)$.

According to Mercer's theorem, every positive definite kernel $K : \Omega \times \Omega \to \mathbb{R}$, where $\Omega \subseteq \mathbb{R}^d$, can be represented in terms of the (positive) eigenvalues λ_n and (normalized) eigenfunctions φ_n of an associated compact integral operator [15], i.e.,

$$K(\mathbf{x}, \mathbf{z}) = \sum_{n=1}^{\infty} \lambda_n \varphi_n(\mathbf{x}) \varphi_n(\mathbf{z}).$$

Since the Gaussian RBF is a positive definite kernel we have

$$\mathrm{e}^{-\varepsilon^2 (x-z)^2} = \sum_{n=1}^{\infty} \lambda_n \varphi_n(x) \varphi_n(z),$$

where the φ_n are orthogonal functions with respect to the weight function $\rho(x) = \frac{\alpha}{\sqrt{\pi}} \mathrm{e}^{-\alpha^2 x^2}$, and

$$\varphi_n(x) = \sqrt{\beta}\, \mathrm{e}^{-\delta^2 x^2} \widetilde{H}_{n-1}(\alpha \beta x). \tag{2}$$

The parameter ε which controls the flatness of the kernel, is called the shape parameter and the parameter α which acts on the same scale as ε, is called the global scale parameter [16,13]. While these two parameters are arbitrary inputs to our