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Radial basis function interpolation in the limit of increasingly flat basis functions

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ABSTRACT

We propose a new approach to study Radial Basis Function (RBF) interpolation in the limit of increasingly flat functions. The new approach is based on the semi-analytical computation of the Laurent series of the inverse of the RBF interpolation matrix described in a previous paper [3]. Once the Laurent series is obtained, it can be used to compute the limiting polynomial interpolant, the optimal shape parameter of the RBFs used for interpolation, and the weights of RBF finite difference formulas, among other things.

1. Introduction

This paper is concerned with the behavior of Radial Basis Function (RBF) interpolation in the limit of increasingly flat functions. In the past, there has been a considerable interest in analyzing this limit [6,8,10,11,14,17,19,20,26] since it leads to accurate interpolants which are effective both for interpolation problems and for solving partial differential equations.

Many RBFs commonly used in interpolation contain a *shape parameter* $\epsilon > 0$ which controls their flatness. As $\epsilon \to 0$, the RBF becomes increasingly flat. In this limit, the interpolation system becomes highly ill-conditioned, but the limit RBF interpolant at any point is well behaved so it converges to a finite number (except in some particular cases). Indeed, Driscoll and Fornberg [6] proved that 1D RBF interpolants converge to Lagrange interpolating polynomials, subject to some easily stated conditions on the RBF. They also observed numerically that in 2D the situation is more complicated, as the limit may not exist and, if it exists, it is a multivariate polynomial that might depend on the node layout and on the used RBF. Existence of the limit polynomial was proved in [18,27]. Conditions on the used RBFs, so that multivariate interpolation converges, have been recently derived in [19,20].

In this work, we analyze the limit of flat RBFs using the framework proposed in [3]. The main ingredient used in our analysis is the Laurent series of the inverse of the interpolation matrix, which we compute using a semi-analytical procedure [3]. The relevant parameter in the Laurent series is $\delta = (\epsilon h)^2$, which is the square of the product of the shape parameter ϵ and a characteristic inter-nodal distance h. If we denote by $r_{i,j}$ the distance between nodes i and j, then the dimensionless distances $r_{i,j}/h$ are of order unity (for details, see, for example, [31]). Multiplying the Laurent series of the inverse of the interpolation matrix by the data at the nodes we obtain a Laurent series for the interpolation coefficients avoiding the ill-conditioning associated to straightforward numerical approaches in the flat RBF limit.

In Ref. [2] we use the Laurent series of the inverse to compute the weights of RBF-FD formulas. In this paper we use the Laurent series of the inverse to approximate the RBF interpolant by a series of interpolation polynomials. This approach has

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several advantages for different issues related to RBF interpolation. We focus our attention in the following three important issues described below where we also note which contributions are novel:

- Derivation of the interpolating polynomial, which is the limit of RBF interpolation when $\delta \to 0$. These polynomials have been derived in some specific cases using symbolic language [6,17]. We not only obtain the leading order polynomial but a series of polynomials in powers of δ. Furthermore, we derive them for any node layout.
- Computation of the optimal value of the shape parameter in RBF interpolation. We propose a new method that makes use of the first two terms of the series of polynomials to obtain the value of δ that minimizes the interpolation error. We consider this new method as one of the main contributions of the paper.
- Derivation of RBF finite difference (RBF-FD) formulas. We use the series of polynomials in powers of δ to obtain the weights of RBF-FD formulas. In this way, we obtain formulas for each weight as a series in powers of δ. We also use these weights to derive exact formulas for the local truncation error.

The results presented in the paper show the usefulness of the Laurent series of the inverse to analyze RBF interpolation in the flat limit. It should be emphasized, though, that for large size problems the bottleneck is the computation of the Laurent series. The semi-analytical procedure that we use [3] is very accurate and efficient compared to its symbolic computation. However, its computational cost grows exponentially with the order of the singularity of the Laurent series. Thus, we can only compute stencils with singularities whose order is not greater than seven. Since the order of the singularity grows with the number of nodes [2] this means that the method is only applicable to a relatively small number of nodes. In fact, it is only possible to compute the Laurent series of the inverse for 36 nonequispaced nodes or 24 equispaced nodes in 2D, and for 84 nonequispaced nodes or 31 equispaced nodes in 3D. To apply it to large number of nodes would require a much faster procedure to compute the Laurent series.

The paper is organized as follows: Section 2 describes the formulation based on the Laurent series of the inverse and how to compute a Laurent series of polynomials that approximates the RBF interpolant in the limit $\delta \to 0$. Section 3 describes several significant results obtained with the proposed procedure. It is structured into three subsections focused on three main applications: limiting polynomial interpolant, computation of the optimal shape parameter and derivation of RBF-FD formulas. Finally, Section 4 contains the main conclusions of the paper.

2. Formulation

RBF interpolation is a very efficient technique for the approximation of scattered data. The data is approximated in the functional space spanned by a set of translated RBFs $\phi(\| \mathbf{x} - \mathbf{x}_k \|)$, where $\phi(\hat{r})$ is a function that only depends on the distance $\hat{r}_k = \| \mathbf{x} - \mathbf{x}_k \|$ to a node $\mathbf{x}_k$. RBFs often contain a free parameter which greatly influences the accuracy of the RBF approximation. For instance, in the case of multiquadrics ($\phi(\hat{r};\epsilon) = \sqrt{1+\epsilon^2 \hat{r}^2}$) or gaussians ($\phi(\hat{r};\epsilon) = e^{-\epsilon^2 \hat{r}^2}$) the free parameter ϵ, known as *shape* parameter, determines the flatness of the radial basis function; as $\epsilon \to 0$ these functions become increasingly flat near the origin. It is convenient to use dimensionless distances by using a characteristic internodal distance h as the spatial unit. Thus, $\epsilon^2 \hat{r}_k^2 = \epsilon^2 h^2 \frac{\|\mathbf{x}-\mathbf{x}_k\|^2}{h^2} = \delta\, r_k^2$, where $\delta = (\epsilon h)^2$, is the square of the product of the shape parameter ϵ times the inter-nodal distance h, and r_k is the dimensionless distance $\| \mathbf{x} - \mathbf{x}_k \| / h$. With this notation the RBF $\phi(\hat{r};\epsilon)$ is rewritten as $\phi(r;\delta)$.

If the data are given at n nodes $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ in d dimensions, the RBF interpolant is given by

$$s(\mathbf{x};\delta) = \sum_{k=1}^{n} \alpha_k(\delta)\, \phi\left(\frac{\| \mathbf{x} - \mathbf{x}_k \|}{h}; \delta \right) = \sum_{k=1}^{n} \alpha_k(\delta)\, \phi(r_k;\delta), \tag{1}$$

where r_k is the nondimensional distance to node $\mathbf{x}_k$. For given data values $f_i = f(\mathbf{x}_i)$, the interpolation coefficients α_k are obtained by solving the linear system

$$A(\delta)\, \boldsymbol{\alpha}(\delta) = \mathbf{f}, \tag{2}$$

where the entries of the $n \times n$ interpolation matrix are $A_{i,j} = \phi\left(\frac{\| \mathbf{x}_i - \mathbf{x}_k \|}{h}; \delta \right)$, and $\boldsymbol{\alpha}(\delta) = [\alpha_1(\delta)\ \alpha_2(\delta)\ \ldots\ \alpha_n(\delta)]^T$ and $\mathbf{f} = [\ f_1\ \ f_2\ \ldots\ \ f_n\ ]^T$ are n-dimensional column vectors. Equation (2) implies that $s(\mathbf{x};\delta)$ computed in (1) interpolates $f(\mathbf{x})$ at nodes $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$. For many choices of RBFs (including multiquadrics) the system is nonsingular for any arbitrary set of nodes. In fact, Micchelli [22] proved that a sufficient condition to guarantee the nonsingularity is that the interpolation matrix is strictly positive definite. Furthermore, it is well known, that large values of δ lead to well-conditioned linear systems, but the resulting approximation is inaccurate. On the other hand, small values of δ lead to accurate results but the condition number of (2) grows rapidly and, hence, the interpolation coefficients α_k diverge in the limit $\delta \to 0$. However, it has been shown [6] that although the interpolation coefficients diverge, the RBF interpolant itself (1) converges to a finite limit (except in some particular cases). Thus, computing $s(\mathbf{x},\delta)$ from $\mathbf{f}(\mathbf{x})$ is a well-conditioned process, but the intermediate step of computing $\boldsymbol{\alpha}$ is ill-conditioned.

In this paper, we compute the interpolation coefficients by means of the Laurent series of the inverse of the interpolation matrix A, which we derive using the semi-analytical procedure described in [3] for infinitely smooth RBFs. In this way,