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SCATTERED NODE MEHRSTELLENVERFAHREN-TYPE FORMULAS GENERATED FROM RADIAL BASIS FUNCTIONS

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Abstract

In standard equispaced finite difference (FD) formulas, symmetries can make the order of accuracy relatively high compared to the number of nodes in the FD stencil. With *scattered* nodes, such symmetries are no longer available. Thus, the number of nodes in the stencils can be relatively large compared to the resulting accuracy. The generalization of *mehrstellenverfahren* (compact) FD (CFD) formulas that we propose for scattered nodes and radial basis functions (RBFs) achieves the goal of reducing the number of stencil nodes without a similar reduction in accuracy. We analyze the accuracy of these new compact RBF-FD formulas by applying them to some model problems, and study the effects of the shape parameter that arises in, for example, the multiquadric radial function.

Keywords: Radial basis functions, partial differential equations, compact finite difference method, mesh-free

Introduction

An obvious approach for circumventing the geometric inflexibility of the standard finite difference method (FDM) for solving partial differential equations (PDEs) is to allow the nodes of the FD stencils to be placed freely, so that a good discretization of the physical domain of the problem can be obtained. However, this natural *mesh-free* idea raises questions of how the weights of the resulting *scattered* node FD formulas should be computed. It has recently (and what appears to be independently) been proposed by Shu *et al.* (2003), Tolstykh *et al.* (2003), Cecil *et al.* (2004), and the present authors (2003) that RBF interpolants be used for computing these weights. We refer to this idea as the RBF-FD method. The following are some reasons for using RBFs: (1) for the appropriate choice of radial function $\phi(r)$, the RBF interpolation method is well-posed in all dimensions (unlike polynomial interpolation); (2) RBF interpolants can be very accurate at approximating derivatives; and (3) Certain types of radial functions $\phi(r)$ feature a "shape" parameter ε that allows them to vary from being nearly flat ($\varepsilon \to 0$) to sharply peaked ($\varepsilon \to \infty$). The recent work of, for example, Fornberg *et al.* (2002) shows that all classical FD formulas can be recovered by "flat" RBF interpolants (when the nodes are arranged accordingly).

In standard equispaced finite difference (FD) formulas, symmetries can make the order of accuracy relatively high compared to the number of nodes in the FD stencil. With scattered nodes, such symmetries are no longer available. Thus, the number of nodes in

the stencils can be relatively large compared to the resulting accuracy. To circumvent this problem, we propose a generalization of compact finite difference (CFD) formulas first introduced by Collatz (1960). The basic idea behind this method is to keep the stencil size fixed and to also include in the FD formula a linear combination of derivatives of u at surrounding nodes. In the case of 1-D and equispaced nodes, the weights for these CFD formulas are typically derived using Padé approximants. For scattered nodes in one and higher dimensions, and for RBFs, this Padé approach is no longer available. Instead, we propose a method based on Hermite RBF interpolation.

Without loss of generality, we limit the discussion to RBF-FD and RBF-CFD formulas for the d-dimensional Laplacian ∇^2.

Hermite RBF interpolation

Since the RBF-CFD formulas are ultimately obtained from Hermite RBF interpolants, we review in this section a method for solving the Hermite interpolation problem. We note that the standard RBF-FD formulas are ultimately obtained from standard RBF interpolants, which turn out to be a special case of Hermite RBF interpolants.

Let σ be a vector containing some combination of $m \leq n$ distinct numbers from the set $\{1, \ldots, n\}$. Given a set of distinct data points $\underline{x}_i \in \mathbb{R}^d$, $i = 1, \ldots, n$, and corresponding (scalar) data values $u(\underline{x}_i)$, $i = 1, \ldots, n$, and $\nabla^2 u(\underline{x}_{\sigma_i})$, $i = 1, \ldots, m$, the Hermite RBF interpolation method we consider is to find an interpolant of the form

$$s(\underline{x}) = \sum_{i=1}^{n} \lambda_i \phi(\|\underline{x} - \underline{x}_i\|) \; + \sum_{j=1}^{m} \alpha_j \nabla^2 \phi(\|\underline{x} - \underline{x}_{\sigma_j}\|) \; + \beta \; . \tag{1}$$

Here $\phi(r)$ is some *radial* function and $\|\cdot\|$ is the standard Euclidean norm. This method is similar to the Hermite-Birkhoff method proposed by Wu (1992). Imposing the Hermite interpolation constraints and the additional constraint $\sum_{i=1}^{n} \lambda_i = 0$ leads to the following symmetric linear system of equations (in block form)

$$\underbrace{\left[\begin{array}{c|c|c} \Phi & \nabla^2\Phi & 1 \\ \hline \nabla^2\Phi & \nabla^4\Phi & 0 \\ \hline 1 & 0 & 0 \end{array}\right]}_{A} \left[\begin{array}{c} \lambda \\ \hline \alpha \\ \hline \beta \end{array}\right] = \left[\begin{array}{c} u \\ \hline \nabla^2 u \\ \hline 0 \end{array}\right] \; . \tag{2}$$

For the appropriate choice of ϕ, A is guaranteed to be non-singular (Sun 1994). Note that for $m = 0$, the Hermite problem reduces to the standard RBF interpolation problem.

In this study, we focus on the multiquadric (MQ) radial function, $\phi(r) = \sqrt{1 + (\varepsilon r)^2}$, since it can produce very accurate interpolants, and it features a free shape parameter ε that can be adjusted to significantly improve the resulting accuracy of the interpolants. We note also that the linear system (2) is guaranteed to be non-singular for the MQ radial function (and ε non-zero).

RBF-FD Formulation

In this section we describe how to generate the RBF-FD and RBF-CFD formulas. Without loss of generality, we consider a stencil consisting of n (scattered) nodes $\underline{x}_1, \ldots, \underline{x}_n$ and are interested in approximating $\nabla^2 u(\underline{x}_1)$. Here we let $\nabla^2 u(\underline{x}_i) := \nabla^2 u(\underline{x})|_{\underline{x}=\underline{x}_i}$.

For RBF-FD formulas the goal is to find weights c_i such that, $\nabla^2 u(\underline{x}_1) \approx \sum_{i=1}^{n} c_i u(\underline{x}_i)$. This is accomplished by solving the linear system

$$A[c|\mu]^T = \Big[\underbrace{\nabla^2\phi(\|\underline{x}-\underline{x}_1\|) \quad \cdots \quad \nabla^2\phi(\|\underline{x}-\underline{x}_n\|)}_{B(\underline{x})} \Big| \, 0 \, \Big]^T , \tag{3}$$

where A is the matrix in (2) (with $m = 0$) and μ is a dummy value related to β in (1).

For the RBF-CFD formulas the goal now is to increase the accuracy of the approximation without increasing the stencil size. We accomplish this by using nodes where u and $\nabla^2 u$ are given exactly. Let σ be a vector containing some combination of $0 < m < n$ distinct numbers from the set $\{2, \ldots, n\}$, then we seek to find weights c_i and $\widetilde{c}_{\sigma_j}$ such that $\nabla^2 u(\underline{x}_1) - \sum_{j=1}^{m} \widetilde{c}_{\sigma_j} \nabla^2 u(\underline{x}_{\sigma_j}) \approx \sum_{i=1}^{n} c_i u(\underline{x}_i)$. This is accomplished by solving the linear system

$$A[c|\widetilde{c}|\mu]^T = \Big[\; B(\underline{x}) \; \Big| \; \nabla^4\phi(\|\underline{x}-\underline{x}_{\sigma_1}\|) \quad \cdots \quad \nabla^4\phi(\|\underline{x}-\underline{x}_{\sigma_m}\|) \; \Big| \; 0 \; \Big]^T , \tag{4}$$

where A is the matrix in (2) and $B(\underline{x})$ is given in (3).

For small (in magnitude) values of the shape parameter ε, the linear systems (3) and (4) will be extremely ill-conditioned. To bypass this problem, we use the Contour-Padé algorithm (Fornberg and Wright 2004), which allows for the stable computation of the RBF-FD and RBF-CFD weights for all $\varepsilon \geq 0$.

Application: Poisson's equation

To illustrate the improved accuracy of the RBF-CFD formulas, we apply them to the model problem

$$\nabla^2 u = f \;\; \text{in } \Omega = \big\{(x,y) \,|\, x^2 + y^2 < 1\big\} \;\; \text{and} \;\; u = g \;\; \text{on } \partial\Omega \, . \tag{5}$$

Note that $\nabla^2 u$ is given analytically as f in the interior. For the experiment that follows, f and g are computed from the known solution

$$u(\underline{x}) = u(x,y) = \frac{25}{25 + (x-0.2)^2 + 2y^2} \, . \tag{6}$$

The domain is discretized using the $N = 200$ points shown in Figure 1 (a). To measure the error (which depends on ε), we use $E(\varepsilon) = \max_{i=1,\ldots,N} |\overline{u}(\underline{x}_i, \varepsilon) - u(\underline{x}_i)|$ (i.e., the max norm), where $\overline{u}$ is the approximate solution. We call the ε where $E(\varepsilon)$ reaches a minimum the "optimal" ε.

Figure 1 (b) contains the results using the $n = 9$ ($m = 0$) node RBF-FD formulas, and the RBF-CFD formulas using $n = 9$ $m = 5$, and $n = 10$ $m = 9$. Looking at the error for the standard $n = 9$ solution and the compact $n = 9$ $m = 5$ solution, we see that the accuracy is vastly improved. As we should expect, the accuracy can be further improved by increasing n and m, as illustrated by the $n = 10$ $m = 9$ solution. For this example, however, any improvements appear to be lost for ε approximately > 0.5. The figure also illustrates that the optimal value of ε is small (in magnitude), and nonzero, as is typically the case for the RBF interpolation problem. Also included in the figure (see the dotted lines) are the results for the standard FD solutions based on a uniform

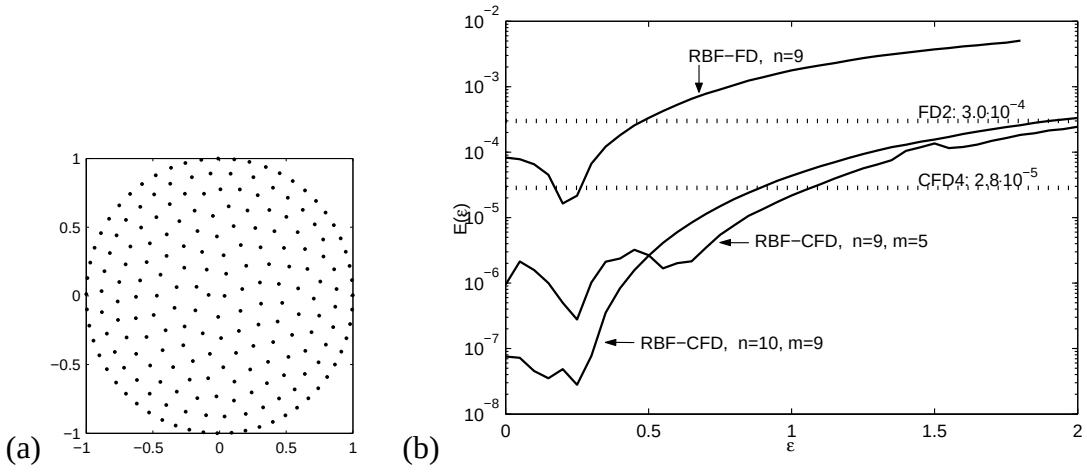

Figure 1: (a) 200 point unstructured discretization of the unit disk. (b) The error as a function of ε for various numerical solutions of (5).

polar mesh with approximately the same number of boundary and interior points as the unstructured mesh. FD2 marks the results for the standard 5-node second-order FD scheme, while CFD4 marks the results for the standard compact 9-node fourth-order FD scheme. Comparing the non-compact FD2 and $n = 9$ RBF-FD solution, we see that approximately for $\varepsilon < 0.48$, the RBF solution is clearly better. Comparing the CFD4 solution and the $n = 9$ $m = 5$ RBF-CFD solution, which both happen to use the same number of nodes and derivative values in their respective stencils, we see that the RBF solution is better for all values of ε approximately < 1.05.

In all cases, the RBF-FD and RBF-CFD solutions to this problem were computed using successive over-relaxation (SOR). Once the optimal relaxation parameter was found, this iterative method turned out to be quite computationally effective.

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