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Radial basis functions for solving differential equations: Ill-conditioned matrices and numerical stability

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ABSTRACT

High-order numerical methods for solving differential equations are, in general, fairly sensitive to perturbations in their data. A previously proposed radial basis function (RBF) method, namely an integrated multiquadric scheme (IMQ), is applied to two-point boundary value problems whose solutions exhibit thin boundary layers. As frequently observed among RBF methods, the matrices arising are ill-conditioned, in this paper to the point of numerical singularity. The sensitivity of the method to perturbations and round-off error is investigated, and evidence is provided that perturbations are not nearly as strongly amplified as suggested by the large condition numbers of the matrices used in the computation.

1. Introduction

Many methods exist for solving boundary value problems (BVPs). The efficacy of each method is largely dependent on the problem itself. Problems more difficult to solve numerically, such as those with interior or boundary layers, will require a large number of discretization points for good resolution. In situations such as these, higher order methods, which depend on a problem's global information to converge to a solution, can be very effective for finding solutions. A method introduced in [1] uses coordinate stretching and the Chebyshev spectral collocation method for a good resolution of boundary layers. By using a transformed boundary value problem, as in [1], more collocation points can be placed in the boundary layer without causing numerical difficulty.

Kansa [2,3] introduced the method of meshless radial basis functions (RBFs) for the solution of differential equations in 1990. One of the most powerful RBF methods is based on Hardy's multiquadric basis functions (MQ) [4]. These methods, however, appear to be notoriously unstable even with a relatively coarse discretization. As suggested in [5], we consider the MQ Integral Formulation (IMQ) with the transformations used in [1]. The matrices arising from this scheme are so ill-conditioned [6] that its high accuracy, as shown in Section 5, would seem surprising. We saw similar results for a spectral collocation method, discussed in [7]. The ill-conditioning of spectral differentiation matrices (and matrices associated with the RBF method) is well known. In general, however, this ill-conditioning does not manifest itself in a loss of accuracy, a fact that was probably first observed by Berrut [8].

In the context of radial basis functions the phenomenon is also known as Schaback's "principle of uncertainty" [9]. Essentially this principle asserts that one cannot have well-conditioned matrices in RBF methods and a small approximation error at the same time. It is also well known in the RBF community that, in general, the problems going from data to expansion

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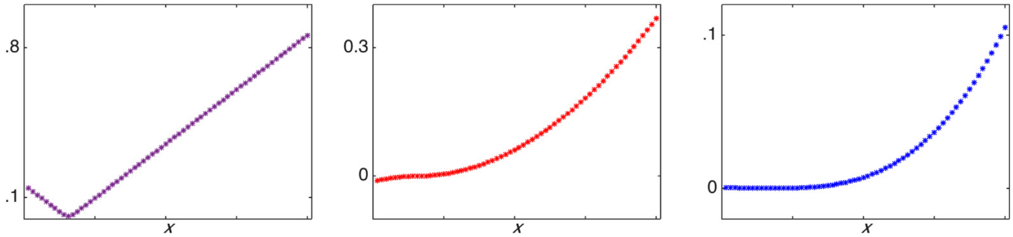

Fig. 1. $\psi_{10}(x)$, $\psi'_{10}(x)$, $\psi''_{10}(x)$.

coefficients, and from expansion coefficients to solution values are both ill-conditioned, but the mathematical problem of going directly from data to the solution values is well-conditioned. In this paper, we will consider whether, and how, perturbations in data are amplified by the IMQ method to the extent suggested by the ill-conditioning of the matrices used in the computation. Our analysis sheds light on the mechanism by which RBF methods achieve high accuracy despite the occurrence of highly ill-conditioned matrices, and the interplay between the two main steps of the algorithm. Sections 5–7 expand on the idea of "effective condition numbers" introduced previously in the literature (see, e.g., [10,11]).

Lastly, we are only looking at one-dimensional problems here, as the purpose of the paper is to explain and illustrate issues of numerical stability. One should expect to observe the same phenomena in higher dimensions, where RBF methods perform very well.

The paper is organized as follows. In Section 2 we describe the Integrated Multiquadric RBF method. Section 3 introduces the model problems for our computations. Section 4 introduces the domain transformations which allow resolution of very thin boundary layers. Section 5 contains a discussion on the condition number of a generic matrix and looks at worst and average case scenarios. Sections 6–7 present our main analysis and results.

2. IMQ scheme for solving BVPs

Consider the singularly perturbed two-point boundary value problem (BVP)

$$\epsilon z''(x) + p(x)z'(x) + q(x)z(x) = f(x), \quad a < x < b, \tag{1}$$

$$z(a) = \alpha, \qquad z(b) = \beta, \tag{2}$$

where $\epsilon > 0$ denotes a fixed (small) constant. We approximate the unknown function $z(x)$ by a linear combination of basis functions $\psi_1, \ldots, \psi_N, 1, \ldots, x^{M-1}$, i.e.,

$$z(x) \approx z^c(x) = \sum_{j=1}^{N} \lambda_j \psi_j(x) + \sum_{\ell=1}^{M} \lambda_{N+\ell} x^{\ell-1}. \tag{3}$$

The basis functions (called integrated multiquadrics) $\psi_j(x)$ are obtained by twice integrating Hardy's multiquadrics [4] $\chi_j(x) = \sqrt{(x-x_j)^2 + c_j^2}$. Hence they have the following form [5] (see Fig. 1):

$$\psi_j(x) = \frac{1}{6}\chi_j(x)(x-x_j) + \frac{c^2}{2}[\ln(\chi_j(x) - (x-x_j)) - \chi_j(x)]$$

with derivatives

$$\psi'_j(x) = \frac{1}{2}\chi_j(x)(x-x_j) + \frac{c^2}{2}\ln(\chi_j(x) + (x-x_j)),$$
$$\psi''_j(x) = \chi_j(x).$$

M is some positive integer. We must also specify N centres x_j and the shape parameter c_j; we use equispaced points for the former. We use the constant shape parameter $c_j = c = .815 \times \text{mean}(d_k)$ suggested by Hardy [4], where d_k is the distance from the kth point to its nearest neighbour, and $\text{mean}(d_k) = \frac{1}{N}\sum_{k=1}^{N} d_k$ is the average of those distances. This may not be the optimal choice for the shape parameter (e.g., [12,13]), but we stayed with this choice for consistency with the results in [5].

Effectively, in the IMQ method we use the Hardy MQ basis to approximate $z''(x)$ instead of $z(x)$, which provides a higher degree of smoothness.

We determine the coefficients λ_j via collocation, i.e., we require $z^c(x)$ to exactly satisfy Eq. (1) at all N centres x_j which serve as collocation points, as well as the boundary conditions (2). With $M = 2$ we have enough degrees of freedom in the numerical approximation $z^c(x)$ to enforce all collocation and boundary conditions. Collocating the BVP (1) at all N centres