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Better bases for radial basis function interpolation problems

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ABSTRACT

Radial basis function interpolation involves two stages. The first is fitting, solving a linear system corresponding to the interpolation conditions. The second is evaluation. The systems occurring in fitting problems are often very ill-conditioned. Changing the basis in which the radial basis function space is expressed can greatly improve the conditioning of these systems resulting in improved accuracy, and in the case of iterative methods, improved speed, of solution. The change of basis can also improve the accuracy of evaluation by reducing loss of significance errors. In this paper new bases for the relevant space of approximants, and associated preconditioning schemes are developed which are based on Floater's mean value coordinates. Positivity results and scale independence results are shown for schemes of a general type. Numerical results show that the given preconditioning scheme usually improves conditioning of polyharmonic spline and multiquadric interpolation problems in $\mathcal{R}^2$ and $\mathcal{R}^3$ by several orders of magnitude. The theory indicates that using the new basis elements (evaluated indirectly) for both fitting and evaluation will reduce loss of significance errors on evaluation. Numerical experiments confirm this showing that such an approach can improve overall accuracy by several significant figures.

1. Introduction

Radial basis function interpolation involves two stages. The first is fitting, solving a linear system corresponding to the interpolation conditions. The second is evaluation. In this paper we introduce new bases for radial basis interpolation problem which lead to a computationally inexpensive method for preconditioning the linear systems associated with fitting. The new basis, when evaluated indirectly, also greatly improves the accuracy of evaluation of the fitted RBF (radial basis function). We also explore positivity properties of the basis.

Radial basis functions have enjoyed great success in a wide variety of data fitting applications such as surface modelling from point clouds, custom manufacture of artificial limbs, ore grade estimation, and flow modelling. They are particularly advantageous when the data is scattered rather than gridded, the former situation occurring frequently with geophysical data. Unfortunately, as is well known, the matrix of the usual formulation of radial basis function interpolation problems in terms of the natural basis is frequently badly conditioned, even when the number of nodes is small. Indeed many authors have commented on the numerical difficulties that solving this system presents [1–5]. In this paper we develop a computationally inexpensive change of basis based on Floater's mean value coordinates. In the planar case forming the differences underlying the change of basis requires only $\mathcal{O}(N \log N)$ operations, where N is the number of interpolation nodes. This leads naturally to an inexpensive preconditioning method for the interpolation system.

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A radial basis function (RBF) with centres $\mathcal{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}$ is a function of the form

$$s(\cdot) = \sum_{i=1}^{N} \lambda_i \Phi(\cdot - \boldsymbol{x}_i) + c_1 p_1(\cdot) + \cdots + c_\ell p_\ell(\cdot), \tag{1}$$

where Φ is a fixed, usually radial, function and $\{p_1, \ldots, p_\ell\}$ is a basis for π^d_{k-1}. Often the side conditions

$$\sum_{i=1}^{N} \lambda_i q(\boldsymbol{x}_i) = 0, \quad \text{for all } q \in \pi^d_{k-1}, \tag{2}$$

are imposed. These can be viewed either as taking away the extra degrees of freedom created by the polynomial part in (1), or alternatively of enforcing some decay near infinity.

Given a set of data values $\{f_1, \ldots, f_N\}$ corresponding to the centres $\mathcal{X}$, the interpolation problem is to find a function of the form (1) satisfying the side conditions (2) and the interpolation conditions

$$s(\boldsymbol{x}_i) = f_i, \quad 1 \le i \le N.$$

Thus, the standard (pointwise) interpolation problem can be written in matrix form as

$$\begin{bmatrix} A & P \\ P^T & O_\ell \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \boldsymbol{c} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{0} \end{bmatrix}, \tag{3}$$

where 0_ℓ is the $\ell \times \ell$ zero matrix,

$$A_{ij} = \Phi(\boldsymbol{x}_i - \boldsymbol{x}_j), \qquad P_{ij} = p_j(\boldsymbol{x}_i), \tag{4}$$

and $\boldsymbol{f} = [f_1, \ldots, f_N]^T$.

We will need the following definitions.

Definition 1.1. A set of linear functionals μ_i, $1 \le i \le m$ will be called unisolvent for π^d_{k-1} if

$$q \in \pi^d_{k-1} \quad \text{and } \mu_j(q) = 0 \text{ for all } 1 \le j \le m \text{ implies } q \text{ is the zero polynomial.}$$

A set of points $\mathcal{X}$ is said to be unisolvent for π^d_{k-1} when the corresponding set of point evaluations has this property.

Definition 1.2. A continuous function $\Phi : \mathcal{R}^d \to \mathcal{R}$ will be called (pointwise) conditionally positive definite of order k on $\mathcal{R}^d$ if

(i) Φ is even.
(ii) For all choices of a positive integer N and of a set $\mathcal{X}$ of N distinct points in $\mathcal{R}^d$, the quadratic form $\boldsymbol{\lambda}^T A \boldsymbol{\lambda}$ is nonnegative for all vectors $\boldsymbol{\lambda}$ such that

$$\sum_{j=1}^{N} \lambda_j q(\boldsymbol{x}_j) = 0, \quad \text{for all } q \in \pi^d_{k-1}. \tag{5}$$

Φ is called strictly conditionally positive definite of order k if the inequality above is strict whenever $\boldsymbol{\lambda} \neq \boldsymbol{0}$.

It is well known that the matrix

$$A_\Phi = \begin{bmatrix} A & P \\ P^T & O \end{bmatrix} \tag{6}$$

of the usual formulation (3) of the interpolation problem is invertible when Φ is strictly conditionally positive (negative) definite of order k, and the points $\mathcal{X}$ are unisolvent for π^d_{k-1}.

The paper is arranged as follows. In Section 2 a general framework for preconditioning based upon a *complete set of differences* is set out. In Section 3 the framework is applied in the example case of natural cubic spline interpolation in $\mathcal{R}^1$. In Section 4 some positivity and decay properties of basis functions Ψ_j generated by difference preconditioning are discussed. In Section 5 scale independence properties of the preconditioned problem are shown. In Section 6 the specifics of a difference preconditioner based on mean value coordinates are presented. In Section 7 numerical results related to the condition numbers seen when the method is applied to random sets of centres are presented. Finally, in Section 8 we present both theory and numerics showing that the new basis significantly improves accuracy in the combination of fitting and evaluation. A key idea in this section is to evaluate the new basis elements indirectly, rather than directly via the $\Phi(\cdot - \boldsymbol{x}_j)$'s.

2. A general framework for preconditioning

In this section we consider a general framework for preconditioning RBF interpolation problems based on a strictly conditionally positive definite Φ.