A multigrid-type method for thin plate spline interpolation on a circle

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Abstract

We consider the problem of thin plate spline interpolation to n equally spaced points on a circle, where the number of data points is sufficiently large for work of $\mathcal{O}(n^3)$ to be unacceptable. We develop an iterative multigrid-type method, each iteration comprising $ngrid$ stages, and n being an integer multiple of $2^{ngrid-1}$. We let the first grid, V_1, be the full set of data points, V say, and each subsequent (coarser) grid, V_k, $k = 2, 3, \ldots, ngrid$, contain exactly half of the data points of the preceding (finer) grid, these data points being equally spaced.

At each stage of the iteration, we correct our current approximation to the thin plate spline interpolant by an estimate of the interpolant to the current residuals on V_k, where the correction is constructed from Lagrange functions of interpolation on *small local subsets* of p data points in V_k. When the coarsest grid is reached, however, then the interpolation problem is solved exactly on its $q = n/2^{ngrid-1}$ points. The iterative process continues until the maximum residual does not exceed a specified tolerance.

Each iteration has the effect of premultiplying the vector of residuals by an $n \times n$ matrix R, and thus convergence will depend upon the spectral radius, $\rho(R)$, of this matrix. We investigate the dependence of the spectral radius on the values of n, p, and q. In all the cases we have considered, we find $\rho(R) \ll 1$, and thus rapid convergence is assured.

1 Introduction

Let f be a function from $\Re^2$ to $\Re$ which has square integrable second derivatives, and let $V = \{\underline{x}_i : i = 1, 2, \ldots, n\}$ be a finite set of points in $\Re^2$ which are all different and which are not collinear. Then the thin plate spline interpolant to f on V is the function s, which minimises the integral

$$I(s) = \int_{\Re^2} \left(\frac{\partial^2 s}{\partial x^2}\right)^2 + 2\left(\frac{\partial^2 s}{\partial x\,\partial y}\right)^2 + \left(\frac{\partial^2 s}{\partial y^2}\right)^2 d\underline{x}, \tag{1.1}$$

subject to the interpolation conditions

$$s(\underline{x}_i) = f(\underline{x}_i), \qquad i = 1, 2, \ldots, n. \tag{1.2}$$

It is known, see Duchon [5], that $s(\underline{x})$ has the form

$$s(\underline{x}) = \sum_{i=1}^{n} \lambda_i\, \phi_i(\underline{x}) + p(\underline{x}), \qquad \underline{x} \in \Re^2, \tag{1.3}$$

where

$$\phi_i(\underline{x}) = \|\underline{x} - \underline{x}_i\|_2^2 \log \|\underline{x} - \underline{x}_i\|_2, \tag{1.4}$$

where

$$p(\underline{x}) = c_1 + c_2 x + c_3 y \tag{1.5}$$

is a linear polynomial, and where the parameters, $\{\lambda_i : i = 1, 2, \ldots, n\}$, satisfy the equations

$$\left.\begin{array}{r} \sum_{i=1}^{n} \lambda_i = 0 \\[2ex] \sum_{i=1}^{n} \lambda_i\, \underline{x}_i = \underline{0} \end{array}\right\}. \tag{1.6}$$

Denoting by A the $n \times n$ symmetric matrix with elements

$$A_{ij} = \phi_i(\underline{x}_j), \qquad i, j = 1, 2, \ldots, n, \tag{1.7}$$

and by P the $n \times 3$ matrix whose i-th row is the vector $[\ 1 \quad x_i \quad y_i\ ]$, we see that equations (1.2) and (1.6) provide the $(n+3) \times (n+3)$ linear system

$$\left.\begin{array}{r} A\,\underline{\lambda} + P\underline{c} = \underline{f} \\[2ex] P^T\underline{\lambda} = \underline{0} \end{array}\right\}, \tag{1.8}$$

which defines uniquely the parameters $\{\lambda_i : i = 1, 2, \ldots, n\}$ and the coefficients $\{c_i : i = 1, 2, 3\}$ of the linear polynomial $p(\underline{x})$.

Several papers, for example Sibson and Stone [7] and Beatson and Powell [2], address the solution of this linear system. In particular, if $\underline{v} \in \Re^n$ is a nonzero vector in the null space of P^T, then $\underline{v}^T A\, \underline{v}$ is positive; and thus, if Q is an $n \times (n-3)$ matrix whose columns span the null space of P^T, one can deduce

$$\underline{\lambda} = Q\underline{\mu}, \tag{1.9}$$

where $\underline{\mu} \in \Re^{n-3}$ is the solution of the $(n-3) \times (n-3)$ positive definite linear system

$$Q^T A Q \underline{\mu} = Q^T \underline{f}. \tag{1.10}$$

After $\underline{\mu}$ has been calculated, the coefficients of the linear polynomial are then given by any three of the interpolation equations (1.2) whose points $\{\underline{x}_i\}$ are not collinear.

The work involved in solving the linear system (1.10) by the Cholesky method, for instance, is of $\mathcal{O}(n^3)$, and we suppose that n is sufficiently large for this amount of computation to be unacceptably high. Instead we develop an iterative multigrid-type method, each iteration comprising a number of stages equal to the number of grids. Our method is motivated by Beatson and Powell [2], who describe a single grid scheme, working on the full set of data points, but using Lagrange functions of interpolation to only small subsets of the data.

In this paper we consider the case where V is the set of n equally spaced points on a circle. On each grid, our method constructs Lagrange functions of interpolation to a subset of the grid points, which, because of the rotational symmetry of the circle, all have the same form. This highly desirable property, which is peculiar to the circle, considerably reduces the amount of preliminary computation (see Section 3). It does not occur for other mesh geometries, for example when V is a square grid.

Of course, in the particular case when V is a set of equally spaced points on a circle, the matrix A, defined in (1.7), is a *circulant matrix*, and therefore the linear system (1.8) can be solved in only $\mathcal{O}(n \log n)$ operations using fast Fourier transforms, see Chapter 3 of Davis [4], which is as efficient as the method we propose. Our method, however, can be adapted to other more general mesh geometries, and here the saving in the amount of computation is considerable.

Our method illustrates well how the combination of multigrid and local approximations to Lagrange functions can provide linear iterative methods which have small spectral radii, and thus guarantee rapid convergence.

2 The multigrid-type method

We initially set

$$s(\underline{x}) := 0, \qquad \underline{x} \in \Re^2, \tag{2.1}$$

and perform the following iterative multigrid-type method.

We let the first grid, V_1, be the full set of data points, V, and each subsequent (coarser) grid, V_k, $k = 2, 3, \ldots, ngrid$, contain exactly half of the data points of the preceding (finer) grid, these $n/2^{k-1}$ points being equally spaced. Thus each iteration comprises $ngrid$ stages, the number of data points, n, being an integer multiple of $2^{ngrid-1}$.

At each stage, $k = 1, 2, \ldots, ngrid - 1$, except the final stage, of an iteration, we correct our current estimate of the thin plate spline interpolant by an estimate of the interpolant to the current residuals on V_k. The estimate is calculated using Lagrange functions of interpolation, each of which is constructed from only a *small local subset* of p data points in V_k. We expect these Lagrange functions to model the true Lagrange functions of interpolation on the full grid, V_k, extremely well; this is due to the excellent localisation properties of the latter functions, see Buhmann [3]. Specifically, the operations of the k-th stage are as follows.

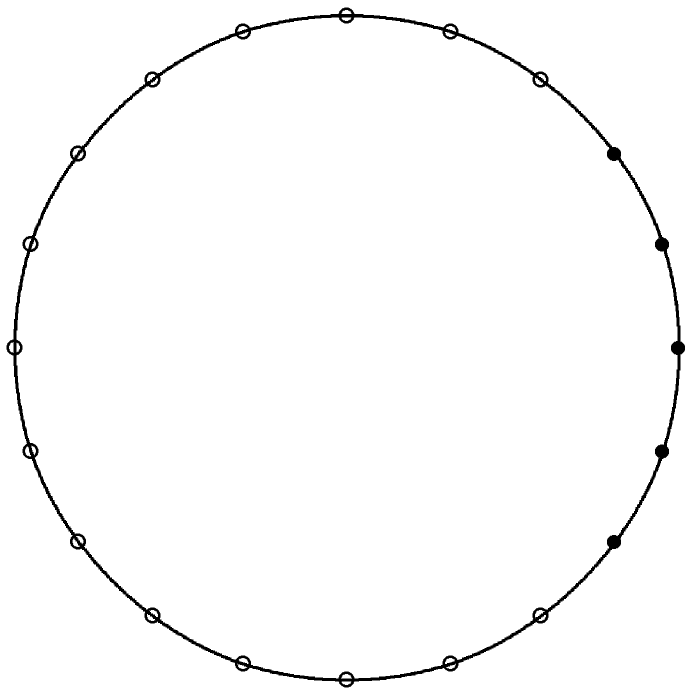

Figure 1: The sets V_k and $\widehat{V}_{kj}$

For each data point, $\underline{x}_j \in V_k$, we define the subset, $\widehat{V}_{kj} \subset V_k$, to be an arc of p adjacent points in V_k whose midpoint is $\underline{x}_j$, where p is an odd number. This is shown in Figure 1, where the solid and hollow circles represent the data points in $\widehat{V}_{kj}$ and $V_k \setminus \widehat{V}_{kj}$, respectively.

We define the sets of indices

$$N_k = \left\{ j : \underline{x}_j \in V_k \right\} \qquad \text{and} \qquad \widehat{N}_{kj} = \left\{ i : \underline{x}_i \in \widehat{V}_{kj} \right\}, \tag{2.2}$$

and we denote by

$$\ell_{kj}(\underline{x}) = \sum_{i \in \widehat{N}_{kj}} \widehat{\lambda}_{kji}\, \phi_i(\underline{x}) + \widehat{p}_{kj}(\underline{x}), \tag{2.3}$$

with

$$\widehat{p}_{kj}(\underline{x}) = \widehat{c}_{kj1} + \widehat{c}_{kj2} x + \widehat{c}_{kj3} y, \tag{2.4}$$

the Lagrange function of thin plate spline interpolation satisfying the Lagrange conditions

$$\ell_{kj}(\underline{x}_i) = \delta_{ij}, \qquad i \in \widehat{N}_{kj}. \tag{2.5}$$

Thus, denoting the current residuals by

$$r_i = f(\underline{x}_i) - s(\underline{x}_i), \qquad i = 1, 2, \ldots, n, \tag{2.6}$$

the k-th stage sets

$$s(\underline{x}) := s(\underline{x}) + \sum_{j \in N_k} r_j \ell_{kj}(\underline{x}), \qquad \underline{x} \in \Re^2. \tag{2.7}$$

As remarked in Section 1, it is only necessary to construct the Lagrange function of interpolation, $\ell_{kj}(\underline{x})$, for a single index, $j \in N_k$; the remaining Lagrange functions are then given by the rotational symmetry of the circle.

At the final stage of an iteration, the interpolation problem is solved *exactly* on the $q = n/2^{ngrid-1}$ points of the coarsest grid, and we correct our current estimate of the interpolant by the exact interpolant to the current residuals on V_{ngrid}. Thus we set

$$s(\underline{x}) := s(\underline{x}) + \tilde{r}(\underline{x}), \tag{2.8}$$

where $\tilde{r}(\underline{x})$ is the thin plate spline function satisfying the interpolation conditions

$$\tilde{r}(\underline{x}_i) = r_i, \qquad i \in N_{ngrid}. \tag{2.9}$$

Thus the residuals are reduced to zero at the data points of the coarsest grid.

The iterative process continues, up to a specified maximum number of iterations, until the maximum residual does not exceed a specified tolerance, typically until $\|\underline{r}\|_\infty < 10^{-10}$.

3 The amount of computation

We now consider the amount of computation of the iterative multigrid-type method described in Section 2. We split the computation into two parts, the first being the preliminary work which is performed once only prior to the commencement of the iterations, and the second being the work done in each iteration.

The preliminary calculation generates the parameters, $\left\{\widehat{\lambda}_{kji} : i \in \widehat{N}_{kj}\right\}$ and $\{\widehat{c}_{kji} : i = 1, 2, 3\}$, of the Lagrange function, $\ell_{kj}(\underline{x})$, for a *single index*, $j \in N_k$, on each grid, $V_1, V_2, \ldots, V_{ngrid-1}$, except the coarsest; and performs the Cholesky factorisation of the matrix $Q^T A Q$, given in (1.10), for thin plate spline interpolation on the coarsest grid, V_{ngrid}. This work is of

$$\mathcal{O}(ngrid\, p^3 + q^3).$$

As remarked in Section 1, the sufficiency of a single Lagrange function on each grid, which is peculiar to the circle, considerably reduces the amount of preliminary computation.

The work done in each iteration involves the updating, on each grid, $V_1, V_2, \ldots, V_{ngrid}$, of the current parameters, $\{\lambda_i : i \in N_k\}$ and $\{c_i : i = 1, 2, 3\}$, of the thin plate spline interpolant, $s(\underline{x})$, and the values of the residuals, $\{r_i : i \in N_{k+1}\}$, required by the next stage of the iteration, the values of all the residuals, $\{r_i : i = 1, 2, \ldots, n\}$, being updated at the final stage of each iteration. This work is of

$$\mathcal{O}(n\, \log n + np + q^2),$$

using the truncated Laurent expansion techniques of Powell [6].

Thus we see that the saving in computation achieved using the iterative multigrid-type method is very significant, provided the method converges fast enough. It is this question of convergence which we address in the next section.

4 Convergence

In order to investigate the convergence of the iterative multigrid-type method, described in Section 2, we observe that each iteration has the effect of premultiplying the vector of residuals, $\underline{r}$, by an $n \times n$ matrix, R, to give

$$\underline{r} := R\underline{r}, \tag{4.1}$$

and that we can write this matrix, R, as the product of $ngrid$ $n \times n$ matrices, R_k, $k = 1, 2, \ldots, ngrid$, such that

$$R = R_{ngrid} R_{ngrid-1} R_{ngrid-2} \ldots R_2 R_1, \tag{4.2}$$

where the k-th stage of each iteration has the effect of premultiplying the current vector of residuals by R_k.

To see this, we note that the application of R_k, $k = 1, 2, \ldots, ngrid - 1$, to the vector of residuals gives

$$r_i := r_i - \sum_{j \in N_k} r_j \ell_{kj}(\underline{x}_i), \qquad i = 1, 2, \ldots, n, \tag{4.3}$$

which follows from (2.7), and that this also holds for $k = ngrid$, where each Lagrange function, $\ell_{ngrid\,j}(\underline{x})$, $j \in N_{ngrid}$, satisfies the Lagrange conditions

$$\ell_{ngrid\,j}(\underline{x}_i) = \delta_{ij}, \qquad i \in N_{ngrid}. \tag{4.4}$$

Thus the rate of convergence of the method depends upon the size of the spectral radius, $\rho(R)$, of the matrix R. We have calculated the spectral radius for a range of values of n, p, and q, and these spectral radii are given in Table 1.

For $n = 160$, $n = 320$, $n = 640$, and $n = 1280$, we have picked $p = 5$, $p = 9$, $p = 17$, and $p = 33$, each new value of p doubling the lengths of the arcs, $\widehat{V}_{kj}$, $j \in N_k$, $k = 1, 2, \ldots, ngrid - 1$. We find that $\rho(R)$ increases when we increase p from $p = 5$ to $p = 9$, which is unexpected, and for which we do not yet have an explanation, but then decreases rapidly for larger values of p. We also find that $\rho(R)$ seems to be independent of q, except when $p = 5$, in which case increasing $ngrid$ by one and halving q does not significantly increase the value of $\rho(R)$. There seems nothing to be gained, therefore, by taking large values of q, with the consequent increase in the amount of computation which that involves.

For fixed p and q, we find that, on doubling the value of n (which increases the value of $ngrid$ by one), we see very little increase in the value of $\rho(R)$. This is very encouraging, and suggests that small values of p and q can provide small values of $\rho(R)$, even when n is very large.

p	q	$n = 160$ $ngrid$	$n = 160$ $\rho(R)$	$n = 320$ $\rho(R)$	$n = 640$ $\rho(R)$	$n = 1280$ $\rho(R)$
5	80	2	0.01218746	0.01216233	0.01215604	0.01286044
5	40	3	0.01218746	0.01216233	0.01283420	0.01371060
5	20	4	0.01218746	0.01283183	0.01370176	0.01397026
5	10	5	0.01248910	0.01347519	0.01392647	0.01404831
9	80	2	0.02254195	0.02256189	0.02256687	0.02256811
9	40	3	0.02254195	0.02256189	0.02256687	0.02256811
9	20	4	0.02254195	0.02256189	0.02256687	0.02256811
9	10	5	0.02254195	0.02256189	0.02256687	0.02256811
17	80	2	0.00431258	0.00433344	0.00433863	0.00433993
17	40	3	0.00431258	0.00433344	0.00433863	0.00433993
17	20	4	0.00431258	0.00433344	0.00433863	0.00433993
33	80	2	0.00073336	0.00075032	0.00075449	0.00075553
33	40	3	0.00073336	0.00075032	0.00075449	0.00075553

Table 1: Values of the spectral radius of the matrix R

In all the cases we have considered, we find $\rho(R) \ll 1$, and thus rapid convergence of the method is assured. When the data points are in general position, rather than a set of equally spaced points on a circle, one should try to minimise the amount of computation, by avoiding large values of p and q, subject to $\rho(R) < 0.1$, say.

5 Final comments

In Section 4, all the numerical examples were for the unit circle with centre at the origin. However, conditions (1.6) on the parameters of the thin plate spline interpolant, and our choice of method, ensure that the results are independent of scaling.

As a final remark, we note that we have had considerable success in adapting the iterative multigrid-type method to other mesh geometries. In particular, Beatson, Goodsell and Powell [1] give some spectral radii for square grids of interpolation points.

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