On the boundary over distance preconditioner for radial basis function interpolation

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Abstract

In this paper we consider the boundary over distance preconditioner for radial basis function interpolation problems. We give both theoretical and numerical results indicating that it performs extremely well.

1 Introduction

Let $\Phi : \mathcal{R}^d \to \mathcal{R}$, $X = \{x_1, \ldots, x_N\}$ be a set of N distinct points in $\mathcal{R}^d$ and f be a real valued function which we can evaluate at least at the x_i's. Define

$$S_{\Phi,X} = \left\{ \begin{array}{l} g : g = \sum_{i=1}^{N} \lambda_i \Phi(\cdot - x_i) \\ \quad \text{where } \sum_{j=1}^{N} \lambda_j q(x_j) = 0, \quad \text{for all } q \in \pi_1^d \end{array} \right\}. \tag{1.1}$$

We consider the problem of finding an element s of $S_{\Phi,X} + \pi_1^d$ satisfying the interpolation conditions

$$s(x_i) = f(x_i), \quad \text{for all} \quad x_i \in X. \tag{1.2}$$

Assume Φ is strictly conditionally positive definite of order 2 (SCPD2) and X is unisolvent for π_1^d. Then there is a unique element of $S_{\Phi,X} + \pi_1^d$ satisfying the interpolation conditions (1.2). This setting includes popular choices of the basic function such as the thin-plate spline, $\Phi(\cdot) = |\cdot|^2 \log|\cdot|$, and minus the ordinary multiquadric, $\Phi(\cdot) = -\sqrt{|\cdot|^2 + c^2}$. In this paper we consider various ways of formulating the interpolation problem, showing in particular that a certain inexpensive change of basis can dramatically improve its conditioning.

The usual way to formulate this problem is in terms of the functions $\{\Phi(\cdot - x_i)\}$ and some basis $\{p_0, p_1, \ldots, p_d\}$ for π_1^d. Then the interpolation conditions together with the side conditions taking away the extra degrees of freedom introduced by the polynomial part can be written as

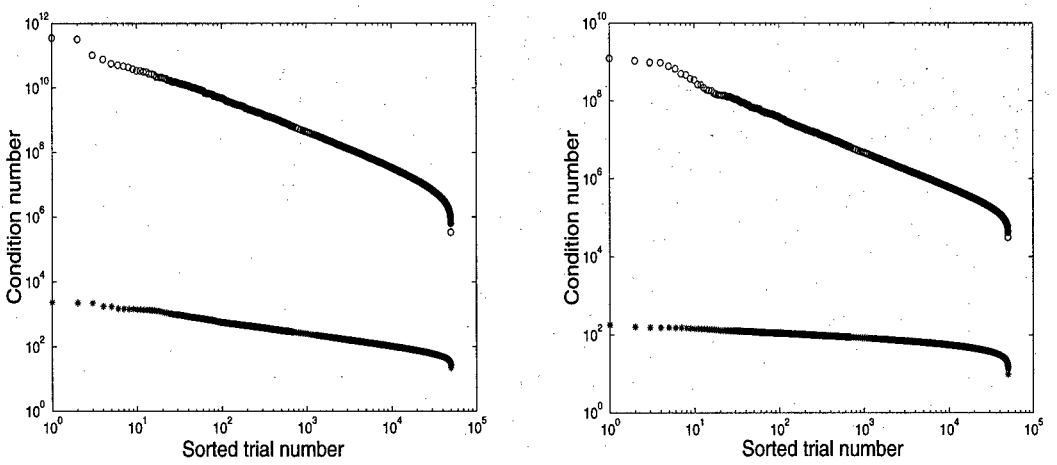
$$A\lambda + Pc = f \qquad \text{and} \qquad P^T\lambda = 0, \tag{1.3}$$

where $A_{ij} = \Phi(x_i - x_j)$, $P_{ij} = p_j(x_i)$, and $f = [f(x_1), \ldots, f(x_N)]^T$. It is well known [3, 4, 5] that the matrix

$$A_\Phi = \begin{bmatrix} A & P \\ P^T & O \end{bmatrix}, \tag{1.4}$$

of this usual formulation 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 [3, 4, 5]. Results of Narcowich and Ward show that conditioning of the system (1.4) depends very heavily on the geometry of the nodes. However, frequently in numerical analysis a change of basis, or other reformulation, can make a highly intractable problem tractable. Hence, our goal is to find an inexpensive but highly effective preconditioner for RBF interpolation systems.

In this paper we establish properties of a preconditioning method for the RBF interpolation equations which was first presented in Sibson and Stone [5]. In the following section we give a detailed account of the preconditioning method. In Section 3 we prove that the construction produces an $N \times (N-3)$ matrix Q whose columns are orthogonal to P, and which is of full rank whenever the nodes X are unisolvent for π_1^2. Finally, Section 4 contains numerical results for different SCPD2 basic functions over a range of data sets and scales. These numerical results show that using this inexpensive $\mathcal{O}(N \log N)$ flop preconditioner and variants of it, dramatically improves the conditioning of RBF interpolation problems. See Figure 1 below.



(a) Multiquadric basic function.

(b) Thin-plate spline basic function.

FIG. 1. Sorted 2-norm condition numbers of the unpreconditioned matrices, A_Φ, (top) and of the preconditioned matrices, S, (bottom) for fifty thousand random data sets of size one hundred.

2 A preconditioning method

A general approach to preconditioning interpolation problems with SCPD2 basic functions in $\mathcal{R}^2$ [1, 5] is to choose Q as any $N \times (N-3)$ matrix whose columns are orthogonal

to P and has rank $N-3$. Letting $\lambda = Q\mu$ and premultiplying (1.3) by Q^T gives the new system to be solved for μ, or equivalently λ,

$$B\mu = Q^T f \qquad \text{where} \qquad B = Q^T A Q. \tag{2.1}$$

The three polynomial coefficients can then be found by a small subsidiary calculation.

In this section we present the boundary over distance method of Sibson and Stone [5] for constructing the matrix Q. We will prove in the subsequent section that Q has full rank and is orthogonal to P for any set of distinct nodes $X = \{x_1, \ldots, x_N\} \subset \mathcal{R}^2$, which are unisolvent for π_1^2. These properties of Q are well known (see e.g. [1, 5]) to imply that the matrix of the preconditioned system $B = Q^T A Q$ is positive definite. The construction of Q is appealing in that for "interior" points x_j of X it is local. That is, for such points the entries in the j-th column of Q depend only on the geometry of the nodes near x_j and not on any properties of nodes far away.

Choose a closed bounded convex polygonal region W of $\mathcal{R}^2$ such that $X \subset W$. Suppose without loss of generality that $\{x_{N-2}, x_{N-1}, x_N\}$ is unisolvent for π_1^2. We will refer to these points as special points. They are generally chosen so that they are well spread throughout W. In our experience, and that of Sibson and Stone, for typical data sets the choice of special points is not at all critical, as long as the triangle they define has largish area. However, for contrived data sets, such as all but a very few points on a straight line, the choice of special points becomes important. In these cases we have observed that bad choices of special points can lead to large condition numbers. However, the strategy of choosing the three special points to maximise the area of the corresponding triangle has always led to small condition numbers.

The region W is divided into panels by intersecting a Voronoi diagram of the points of X with the region W. We denote this panelling of W by

$$V_W(X) = \bigcup_{i=1}^{N} V_i$$

where V_i is the Voronoi panel about the ith centre and is defined by

$$V_i = \{x \in W : |x - x_i| < |x - x_j|, \quad \text{for all } 1 \le j \le N \text{ with } j \ne i\}.$$

Recall that the locus of points equidistant from two fixed points is the perpendicular bisector of the segment connecting the points. It follows that each Voronoi region is polygonal. Associated with a panel V_i are its edges. These are a finite number of distinct closed line segments of non-zero length. They are the boundaries between different Voronoi panels, or between a Voronoi panel and W^C. The collection of all edges of all the Voronoi panels will be denoted by $\mathcal{E}$.

Definition 2.1 *Two polygonal regions of $\mathcal{R}^2$ will be said to be strongly contiguous if they have a common boundary of non-zero length.*

Definition 2.2 *Two Voronoi regions V_i and V_j will be said to be C-related if there is a sequence*

$$\{V_i, V_{\ell_1}, V_{\ell_2}, \ldots, V_{\ell_m}, V_j\}, \qquad 1 \le i, j, \ell_1, \ldots, \ell_m \le N-3,$$

in which all adjacent pairs are strongly contiguous.

Loosely speaking V_i and V_j are C-related if they are connected by a chain of strongly contiguous pairs. C-related is an equivalence relation on the set $\{V_i\}_{i=1}^{N-3}$ of Voronoi regions of non-special points. Therefore it breaks this set into a finite number of nonempty equivalence classes $\{\mathcal{G}_l : 1 \leq l \leq k\}$.

Lemma 2.3 *Let $\mathcal{G}_\ell$ be any of the equivalence classes above. Then there is at least one Voronoi region V_i in $\mathcal{G}_\ell$ which is strongly contiguous to either W^C or one of $\{V_{N-2}, V_{N-1}, V_N\}$.*

Proof: Consider
$$T = \bigcup_{i:V_i \in \mathcal{G}_\ell} \overline{V_i}\,.$$

This union is a closed bounded connected polygonal set whose boundary can be written as the union of some of the line segments from $\mathcal{E}$. Recall in particular that all these line segments have non-zero length. Pick one line segment $< a, b >$ from the boundary of T. Since it forms part of the boundary of T on one side of it lies a Voronoi region V_i from $\mathcal{G}_\ell$. On the other side lies either W^C or another Voronoi region V_j. In the first case the Lemma is proven. Consider the second case. If $1 \leq j \leq N-3$ then V_i is strongly contiguous to V_j. Consequently, $V_j \in \mathcal{G}_\ell$. This contradicts $< a, b >$ being on the boundary of T. Hence, $N-2 \leq j \leq N$ and the Lemma follows. □

We now detail the construction of the $N \times (N-3)$ matrix Q using boundary over distance weights. Note that because most elements of Q are zero sparse storage of Q requires only $\mathcal{O}(N)$ memory. A non-special point from $\{x_i : 1 \leq i \leq N-3\}$ which has Voronoi tile that is strongly contiguous to W^C will be called a *Voronoi external point.* Define $V_E(X)$ as the set of indices of all Voronoi external points. All other points are referred to as *Voronoi internal points.* The corresponding indices are $V_I(X) = \{1, \ldots, N-3\} - V_E(X)$.

We first consider forming a column of Q for an index, j, such that $j \in V_I(X)$. In this case the panel V_j shares non-trivial edges only with other Voronoi panels and not with W^C. The column is formed using boundary over distance weights, found from the Voronoi diagram. For $j \in V_I(X)$ the boundary over distance weight r_{ij} is

$$r_{ij} = \frac{b(x_i, x_j)}{|x_i - x_j|}, \quad \text{for all } V_i \text{ strongly contiguous to } V_j, \tag{2.2}$$

where $b(x_i, x_j)$ is the length of the boundary between V_i and V_j. For other values of $i \neq j$, r_{ij} is set to zero. In order that column j of Q is orthogonal to constants the diagonal element r_{jj} is specified as

$$r_{jj} = -\sum_{i \neq j} r_{ij}. \tag{2.3}$$

Finally, the jth column of R is scaled by dividing by the area of V_j to obtain the jth column of Q. Note that the column is by construction diagonally dominant, but not strictly so.

If $j \in V_E(X)$ then V_j is stongly contiguous to the complement of W, W^C. The boundary segment corresponds to a Voronoi edge between x_j and an artificial point, the reflection of x_j in the boundary (see Figure 3 in [7]). The reflected point, $\hat{x}_j$, can be

written as a linear combination of the special points, i.e.,

$$\hat{x}_j = \lambda_N x_N + \lambda_{N-1} x_{N-1} + \lambda_{N-2} x_{N-2}, \tag{2.4}$$

where $\lambda_N + \lambda_{N-1} + \lambda_{N-2} = 1$. If V_j has k edges with W^C then k reflected points $\{\hat{x}_j^1, \ldots, \hat{x}_j^k\}$ are required. Associated with each reflected point, $\hat{x}_j^a$, are the coefficients $\{\lambda_N^a, \lambda_{N-1}^a, \lambda_{N-2}^a\}$. The boundary over distance weights for $\hat{x}_j^a$ are partitioned amongst the special points to obtain for all $j \in V_E(X)$ and $i \neq j$

$$r_{ij} = \begin{cases} \frac{b(x_i, x_j)}{|x_i - x_j|}, & V_i \text{ strongly contiguous to } V_j, \\ \sum_{l=1}^{k} \lambda_i^l \frac{b(\hat{x}_j^l, x_j)}{|\hat{x}_j^l - x_j|}, & i \in \{N, N-1, N-2\}. \end{cases} \tag{2.5}$$

Of course, V_j could be strongly contiguous with a Voronoi panel associated with a special point. If this is the case $r_{ij} = \frac{b(x_i,x_j)}{|x_i - x_j|} + \sum_{l=1}^{k} \lambda_i^l \frac{b(\hat{x}_j^l, x_j)}{|\hat{x}_j^l - x_j|}$. Again, for other values of $i \neq j$, r_{ij} is set to zero. Finally r_{jj} is specified as in (2.3) and column j of Q is defined as column j of R scaled by dividing by the area of V_j.

Partition Q as

$$Q = \begin{bmatrix} E \\ F \end{bmatrix}, \tag{2.6}$$

where E is $(N-3) \times (N-3)$. Thus E results from interactions between non-special points, and F those between special and non-special points. Note in the construction above that for $1 \leq i, j \leq N-3$, e_{ij} is non-zero if and only if V_i is strongly contiguous to V_j. Furthermore, note that E is necessarily column diagonally dominant, with strict dominance in column j whenever V_j is strongly contiguous to the Voronoi region of a special point, or to W^C.

Relabelling if necessary we can assume the indices of the Voronoi regions in each of the equivalence classes $\mathcal{G}_i$ form a contiguous subset of $\{1, \ldots, N-3\}$. Similarly, we can also assume that the indices corresponding to any $\mathcal{G}_i$ precede those corresponding to $\mathcal{G}_{i+1}$. Furthermore, by construction if $i \neq j$ none of the regions in $\mathcal{G}_i$ is strongly contiguous with a region in $\mathcal{G}_j$. Thus, corresponding entries in the matrix E constructed using boundary over distance weights and artificial points are zero. That is E is block diagonal with the square matrix E_{ii} on the main diagonal corresponding to the equivalence class of Voronoi regions $\mathcal{G}_i$. More precisely, Q will have form

$$Q = \begin{bmatrix} E_{11} & O & \cdots & O \\ O & E_{22} & \cdots & O \\ \vdots & \vdots & \ddots & \vdots \\ O & O & \cdots & E_{kk} \\ F_1 & F_2 & \cdots & F_k \end{bmatrix}. \tag{2.7}$$

3 Properties of the matrix Q

In this section we establish the fundamental properties of the matrix Q of (2.7). Namely that it is of full rank and that its columns are orthogonal to those of P.

Definition 3.1 *For $m \geq 2$, an $m \times m$ matrix K is irreducible if there does not exist an $m \times m$ permutation matrix P such that*

$$PKP^T = \begin{bmatrix} M_{11} & M_{12} \\ 0 & M_{22} \end{bmatrix},$$

where M_{11} is $r \times r$, M_{22} is $(m-r) \times (m-r)$, and $1 \leq r < m$.

The following result is well known, see for example Varga [6].

Theorem 3.2 *Suppose the square matrix K is irreducible and row (column) diagonally dominant with strict row (column) diagonal dominance in at least one row (column). Then K is invertible.*

Lemma 3.3 *Let X be a finite set of distinct points unisolvent for π_1^2. Let E_{ii} be one of the square blocks from the diagonal of Q constructed in the previous section. Then E_{ii} is invertible.*

Proof: From the construction E_{ii} is column diagonally dominant. Furthermore, by Lemma 2.3 the diagonal dominance is strict for at least one column of E_{ii}. From the definition of the equivalence relation C-related there is a chain of strongly contiguous pairs of Voronoi regions, connecting any two Voronoi regions in $\mathcal{G}_i$. This implies the corresponding entries in E_{ii} are non-zero and hence from [6] Theorem 1.6 E_{ii} is irreducible. It follows from Theorem 3.2 that E_{ii} is invertible. □

Theorem 3.4 *The matrix Q described in Section 2 is orthogonal to P i.e. $Q^T P = O$.*

Proof: Omitted, see [2] and [7]. □

Theorem 3.5 *Let X be a set of distinct points unisolvent for π_1^2. Let Q be formed by the construction in Section 2 and $A_{ij} = \Phi(x_i - x_j)$ where Φ is strictly conditionally positive definite of order 2. Then $B = Q^T A Q$ is positive definite.*

Proof: From Lemma 3.3 each of the matrices E_{ii} occurring in the block partitioning of Q given in Equation (2.7) is invertible. Hence Q has full rank. Also from Theorem 3.4 the columns of Q are orthogonal to the columns of P. Let μ be any non-zero vector in $\mathcal{R}^{N-3}$, and define $\lambda = Q\mu$. Then $\lambda \neq 0$, $P^T\lambda = P^T Q\mu = 0$, and $\mu^T B\mu = \mu^T Q^T A Q\mu = \lambda^T A\lambda$. Hence, by the definition of strictly conditionally positive definite, $\mu^T B\mu > 0$ whenever $\mu \neq 0$ and B is symmetric positive definite. □

Theorem 3.6 *Let Φ be strictly conditionally positive definite of order 2 and such that $\Phi(hx, hy) = h^\gamma \Phi(x, y) + p_h(x - y)$, $h > 0$ with $p_h \in \pi_3^2$. The preconditioned matrix B_h, which corresponds to preconditioning on the point set hX, is a homogeneous function of scale. Thus its condition number and the relative clustering of its eigenvalues are the same over all scales.*

Proof: Omitted, see [7]. □

Theorem 3.6 applies in particular to the usual thin-plate spline, $\Phi(\cdot) = |\cdot|^2 \log|\cdot|$, in $\mathcal{R}^2$.

The extended version of this paper [7] contains a proof that the elements B_{ij} decay like $|x_i - x_j|^{-\kappa}$ when $|x_i - x_j|$ is large. For the multiquadric κ is three and for the thin-plate spline κ is two.

Definition 3.7 *The preconditioned matrix S is obtained from B by pre-multiplying and post-multiplying B by the diagonal matrix D with ii entry $1/\sqrt{b_{ii}}$.*

4 Numerical results

In this section we present numerical results for the thin-plate spline and multiquadric basic functions. In the following tables the matrix A_Φ is defined in (1.4), B in (2.1), S in Definition 3.7 and the homogeneous matrix, C, is presented in [1]. In Table 1 we show 2–norm condition numbers of matrices for the various preconditioning techniques over seven different scales. It is clear that the algorithm in Section 2 gives a matrix which dramatically improves the conditioning of the interpolation problem. In one case by a factor of 10^{14}! Tables 2 and 3 contain condition numbers of the matrices resulting from applying the preconditioning techniques of this paper for the thin-plate spline and multiquadric basic functions. For $N < 3200$, the entries in the tables are the maximum over one hundred random point sets of size N. For $N = 3200$, the tables contain the maximum over twenty random point sets of size 3200. In all cases the preconditioning results in a smaller condition number. For these basic functions the maximum observed condition number of the scaled preconditioned matrix, S, grows very slowly with N. Certainly there is no numerical evidence of power growth with N.

Scale parameter α	Conventional matrix A_ϕ	Homogeneous matrix C	Preconditioned matrix B	Scaled matrix S
0.001	1.531(11)	1.534(5)	4.905(1)	2.405(1)
0.01	1.544(9)	1.534(5)	4.905(1)	2.405(1)
0.1	1.597(7)	1.534(5)	4.905(1)	2.405(1)
1	3.107(5)	1.534(5)	4.905(1)	2.405(1)
10	1.915(6)	1.534(5)	4.905(1)	2.405(1)
100	1.271(11)	1.534(5)	4.905(1)	2.405(1)
1000	4.006(15)	1.534(5)	4.905(1)	2.405(1)

TAB. 1. Condition numbers for one hundred points in $[0,\ \alpha]^2$ and the thin-plate spline. The point set for scale α is $X_\alpha = \alpha X_1$.

In an attempt to rule out the possibility that our numerical results were flukes due to the small number of 100 experiments we also conducted 50,000 trials with random data sets of size 100. The results of these trials are shown in Figure 1. The maximum condition number, over all trials with the thin-plate spline, for the matrix A_ϕ was 1.2465(9), for matrix C, 1.5750(9) and for matrix S, 1.8066(2). In our experiments the matrix S is always well conditioned. This held even for geometries of centres for which the matrix A_ϕ is very badly conditioned.

To test further the behaviour of S for "bad" configurations of points a similar experiment was run with one thousand trials of one hundred points almost on a circle. The maximum condition numbers of the A matrix, C matrix and S matrix were 1.2885(9), 7.2692(8) and 6.6005(2) respectively over 1000 trials. Even though the Voronoi regions

Number of data points	Conventional matrix A_ϕ	Homogeneous matrix C	Preconditioned matrix B	Scaled matrix S
200	6.555(7)	3.068(7)	1.617(3)	6.028(1)
400	5.675(8)	3.397(8)	1.945(3)	8.946(1)
800	1.960(10)	1.348(10)	2.034(3)	9.775(1)
1600	1.092(10)	8.413(9)	8.099(3)	1.258(2)
3200	4.997(10)	3.783(10)	1.261(4)	1.569(2)

TAB. 2. Maximum condition numbers encountered over a sample of 100 random point sets of size N in $[0,\ 1]^2$ with the thin-plate spline.

Number of data points	Conventional matrix A_ϕ	Preconditioned matrix B	Scaled matrix S
200	2.014(8)	1.532(2)	4.224(1)
400	2.045(10)	5.932(2)	7.669(1)
800	6.641(10)	4.559(2)	5.826(1)
1600	1.554(10)	7.025(2)	5.601(1)
3200	2.477(11)	9.362(2)	6.280(1)

TAB. 3. Maximum condition numbers encountered over a sample of 100 random point sets of size N in $[0,\ 1]^2$ with the multiquadric function, parameter $c = 1/\sqrt{N}$.

are long and thin the matrix S is still well conditioned!

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