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STABLE MULTIQUADRIC APPROXIMATION BY LOCAL THINNING

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Abstract. In this paper our concern is the recovery of a highly regular function by a discrete set X of data with arbitrary distribution. We consider the case of a nonstationary multiquadric interpolant that presents numerical breakdown. Therefore we propose a global least squares multiquadric approximant with a center set T of maximal size and obtained by a new thinning technique. The new thinning scheme removes the local bad conditions in order to obtain $A_{X,T}$ well conditioned. The choice of working on local subsets of the data set X provides an effective solution. Some numerical examples to validate the goodness of our proposal are given.

Keywords: Scattered data, arbitrary distribution, thinning, least squares, non stationary multiquadric approximant.

AMS classification: 65D10, 41A05.

§1. Introduction

In this article we address the problem of recovering a function with high regularity by using a set of data with arbitrary distribution.

It is well known that the radial basis functions (RBF) are a powerful tool for the multivariate approximation from scattered data. Nevertheless the arbitrary distribution of the data can lead to an ill conditioned problem. In fact the standard methods involve the solution of linear systems whose matrices can be ill conditioned also for moderate size.

In the literature we find various approaches to solve the problem of the ill conditioning when RBFs are considered. A wide list of papers can be found in the recent article [2]. Anyway, the techniques developed take into account only the case of samples from quasi uniform distributions.

In the present paper, the reconstruction of the unknown function is provided by a multiquadric (MQ) least squares approximant with the basis functions located at centers, determined such that the collocation matrix is well conditioned in the sense that Matlab does not display a warning that it is close to singular. The procedure to select the centers is studied in order to provide a solution with very good accuracy.

The note is organized as follows: the main result is presented in §4 and it concerns the determination of the set of the centers; and before we give some notations in §2 and we present the least squares approximant by radial basis functions in §3. Finally in §5 we provide some numerical examples that simulate real applicative cases to show the effectiveness of the proposed technique.

§2. Notations

Given $\{(x_j, f_j),\ j = 1, \dots, N\}$ with data sites $x_j \in D \subset \mathbb{R}^2$ and values $f_j = f(x_j) \in \mathbb{R}$ measured from some unknown function $f \in C^\alpha(D)$, $\alpha > 2$, we indicate with X the set of the data sites x_j, $j = 1, \dots, N$, and with $q(X)$ the minimal distance among the X sites. Similarly we name $T := \{t_1, \dots, t_M\}$ a set of distinct points $t_k \in D$ and $q(T)$ the minimal distance among themselves.

We consider the multiquadric function with fixed parameter δ

$$\phi((\cdot - y), \delta) := \left(\|\cdot - y\|_2^2 + \delta^2\right)^{1/2} = \phi_\delta(\cdot)$$

and we denote with $A_{X,X}$ the interpolation matrix with entries $a_{ij} = \phi((x_i - x_j), \delta)$, $x_i, x_j \in X$ and with $A_{X,T}$ a matrix whose entries are $b_{ij} = \phi((x_i - t_j), \delta)$, $x_i \in X$, $t_j \in T$. Let $\mathcal{K}_2(A_{X,X})$ be the spectral condition number.

Given two sets X and T, we define the covering radius according to the l_2 measure of the set T on X

$$r_{TX} = \max_{x_j \in X} d_T(x_j),$$

where

$$d_T(x_j) = \min_{t_k \in T} \|t_k - x_j\|_{l_2}. \tag{1}$$

Another important parameter is the fill distance

$$h_D(X) = \max_{x \in D} d_X(x),$$

where

$$d_X(x) = \min_{x_j \in X} \|x - x_j\|_{l_2}.$$

We observe that, in the case where we consider the generic point $x \in D$ in (1), the fill distance is synonymous of covering radius.

§3. About least squares approximation

We are interested in providing a solution of the least squares problem when we sample a function f on the set $X = \{x_1, \dots x_N\}$ of data sites and consider a second set $T := \{t_1, \dots, t_M\}$, at which we center the multiquadric bases with fixed parameter δ. Let it be $M < N$.

Let the approximant be of the form

$$Q_f(x) = \sum_{j=1}^{M} c_j \phi((x - t_j), \delta), \quad x \in \mathbb{R}^2.$$

The coefficients $\{c_j\}$ are obtained as solution of the least squares problem

$$A_{XT}\mathbf{c} = \mathbf{f},$$

where $\mathbf{f} = \{f_1, \dots, f_N\}$. The system has a unique solution if the matrix $A_{X,T}$ of entries $\{A_{ij} := \phi((x_i - t_j), \delta)\}$, $i = 1, \dots N$, $j = 1, \dots M$, has full rank.

Unfortunately it is not clear how to choose the set T; in fact there is not much mathematical theory to guarantee that this approach is well posed. However, often the least squares method is a valid tool to obtain a global approximation which takes into account the whole information given by the problem. In this connection we want to show by a simple example that it is very important not to discard any datum.

We consider the set X shown in Fig. 6. In this set the presence of two couples, where the points are very close to each other, leads to an unstable interpolation matrix. A possible choice is that of considering for each couple only one point and then to interpolate the data of the new set $\tilde{X}$ whose matrix $A_{\tilde{X},\tilde{X}}$ is stable. In this way, considering Franke's test function, we obtain a maximum error

$$e_\infty = 7.56\ e(-2),$$

computed on a grid 61×61. Otherwise, considering the least squares method with full rank matrix $A_{X,T}$, we obtain a maximum error

$$e_\infty = 3.80\ e(-2).$$

We observe that to consider all the given functional values leads to an accuracy of one order greater than that obtained by stable interpolation.

Therefore, having considered what we have said above, we have developed a wide experimentation in order to find some information about the construction of a set T associated to a full rank matrix $A_{X,T}$, less hard than the theoretical properties given by Quak, Sivakumar and Ward in [9]. On the basis of our experimentation, one can make the conjecture: " the rank of the matrix $A_{X,T}$ mainly depends on the parameter $q(T)$". Such a statement was indicated also by Buhmann in [1].

§4. Determination of the set T

We suppose that the interpolation matrix $A_{X,X}$ presents a numerical breakdown. Therefore, as it is not possible to consider the interpolant, we want to individuate a set T of centers with a size as large as possible such that the matrix $A_{X,T}$ has full rank to provide a least squares approximant.

The first step in the construction of the set T deals with the determination of an upper bound M_0 for the size of T. For this aim, we recall that the numerical stability of the RBF-ϕ interpolation depends on $G_\phi(q(X))$, where $G_\phi : [0, \infty) \to [0, \infty)$ is a monotonically increasing function. It follows that as the size N of the sample increases and $q(X)$ decreases, the spectral condition number $\mathcal{K}_2(A_{X,X})$ grows.

But we observe that, for a given distribution of the sample, the value of N for which the matrix $A_{X,X}$ presents numerical breakdown depends on the function ϕ or on the value assigned to the parameter of those radial bases such as the Gaussian or the multiquadric for example.

For instance, considering the vertices of a regular hexagonal grid as point locations, we note that a fit by Gaussians, with parameter $\epsilon = 1$, quickly leads Matlab to display a warning of matrix close to be singular, as soon as $N > 46$; whereas with the multiquadric basis with parameter $\delta = 1$ the warning is displayed with $N \geq 85$.

The polyharmonic basis functions are more stable. Sizes of the sample of the order of one thousand can be used to interpolate without instability.

Having fixed the multiquadric basis, we must still define which set of points to choose from which to determine the value M_0 that bounds the size of T with the chosen basis. It is natural to require the stability of the solution for the set T, but also an optimal accuracy. So we recall that all the least squares estimates are based on interpolation error estimates.

In the interpolation problem the pointwise error bound depends on the fill distance of the set of the data sites in D. It follows that, to determine the maximum bound of the size for the set T, we have to search a set T_0 of discrete points in D for which on one hand the value $q(T_0)$ is as large as possible and on the other hand the value $h_D(T_0)$ is as small as possible in order to minimize the mesh ratio $\rho_D(T_0) = h_D(T_0)/q(T_0)$. It is known that the optimal set in $\mathbb{R}^2$ is given by the vertices of a regular hexagonal grid, [4].

4.1. Determination of the bound M_0

Our goal is to consider a set T with parameter $h_D(T)$ as small as possible; this is equivalent to look for a set T of cardinality as large as possible, constrained so that A_{TT} is numerically stable.

Having fixed the multiquadric ϕ_δ, we consider a regular hexagonal grid V_l and compute the spectral condition number $\mathcal{K}_2(A_{V_l,V_l})$. Then we decrease the step of the grid V_l and we obtain a new set of vertices V_{l+1} and a new value $\mathcal{K}_2(A_{V_{l+1},V_{l+1}})$. The process goes on, for a value $l = L$ of the index, until we meet the matrix A_{V_L,V_L} numerically unstable.

The set V_L is the one that corresponds to the value of minimal mesh ratio among all the sets of same cardinality: $\rho_D(V_L) = \min \rho_D(T)$, $|T| = |V_L|$. The value L is the upper bound M_0; it corresponds to the optimal distribution of centers, but it is not always suitable to take them, when considering a set X of scattered points with arbitrary distribution. The value of the size M of the set T will be the closer to M_0 the more the distribution of the sample is almost uniform.

4.2. Determination of T: sketch of the procedure

Once the basis ϕ_δ, for which the value M_0 is known, is fixed, the individuation of the set T is worked in two steps. At first we determine a proper subset of X and then we improve its covering radius on X. To construct the proper subset of X we take into account that:

- Coalescent points determine instability and hence matrices of moderate size can be unstable.
- A warning of ill conditioning depends on the value of $q(X)$ but also on the geometry of the points. With respect to this we show the following example to validate the statement. We consider two different small configurations X, both of size 5 that are shown in Fig. 1 and Fig. 2 respectively; we provide the values of $q(X)$ and $\mathcal{K}_2(A_{X,X})$, when interpolating with the multiquadric with parameter ($\delta = 10$).

  In the first case it is $\mathcal{K}_2(A_{X,X}) = 8.62\ e(15)$ and $q_1(X) = 10\ e(-4)$; in the second case it is $\mathcal{K}_2(A_{X,X}) = 1.77\ e(16)$ even if the minimal distance $q_2(X) = 10\ e(-3)$ is larger than $q_1(X) = 10\ e(-4)$.
- A bad local condition involves a bad global condition

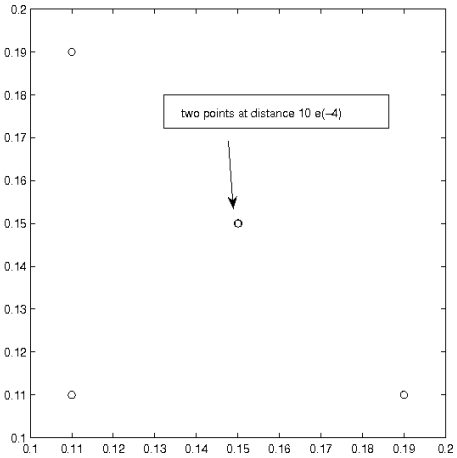

Figure 1:

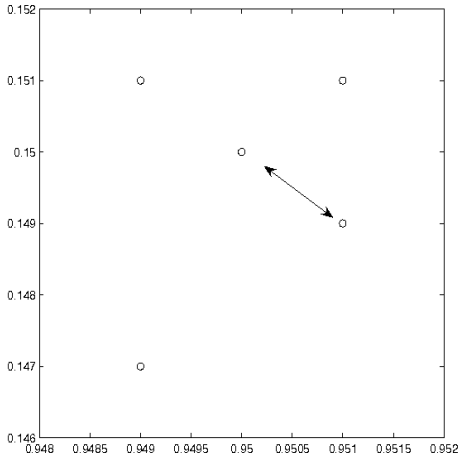

Figure 2:

In the following we sketch the procedure to determine the centers and we refer to [6] for the whole description of the algorithm. For clearness of exposition, we assume that we are in the presence of a sample of size N sampled from uniform distribution.

Using the Delaunay triangulation $\mathcal{D}(X)$, we sort the data sites in a vector $Y = \{y_1, \ldots, y_N\}$ according to the increasing distance from the contiguous points within $\mathcal{D}(X)$. It follows that the last M_0 components of the vector Y correspond to points whose interpoint distances are larger.

We indicate with $Y_0 \coloneqq \{y_{N-M_0+1}, \ldots, y_N\}$ such a vector and we consider for each component $y_k \in Y_0$ its Voronoi cell $V(y_k)$. We calculate the set $Y_0^\star = \{y^\star_{N-M_0+1}, \ldots, y^\star_N\}$ whose components correspond to the barycenters of the sets $X \cap V(y_k),\ k = N - M_0 + 1, \ldots, N$. The vector $Y_0^\star$ has covering radius $r_{Y_0^\star X}$ less than $r_{Y_0 X}$.

By this operation the value of $q(Y_0^\star)$ is larger than $q(X)$; nevertheless $A_{Y_0^\star, Y_0^\star}$ can be unstable due to particular geometries of the data sites. In this last case we consider a subdivision of $Y_0^\star$ in subsets $\{S_j\}$ worked in the following way.

We construct the Delaunay triangulation $\mathcal{D}(Y_0^\star)$ on $Y_0^\star$ and, for each $y_k^\star \in Y_0^\star$, we calculate the average distance

$$\tau_k = 1/n_k \sum_{1}^{n_k} \mathrm{dist}_2(y_k^\star, y_j^\star)$$

from its neighbouring centers. We construct the vector Z whose components $z_k \in Y_0^\star$ are sorted by increasing values of τ_k. The first components of Z correspond to regions of D with largest density of $Y_0^\star$ points.

Let m be fixed and let us start with the first component z_1 of Z to determine the $(m-1)$ points $y_i^\star \in Y_0^\star$ closest to z_1 according to dist_∞. Let us indicate with S_1 such a set. Successively we determine the subsets S_j in the same way by considering the component $z_j \in Z \setminus \cup_{k=1}^{j-1} S_k$ and by individuating the $(m-1)$ points $y_j^\star \in Y_0^\star \setminus \cup_{k=1}^{j-1} S_k$ closest to z_j. The process ends in a finite number of steps.

For each subset S_j we evaluate the condition $\mathcal{K}_2(A_{S_j,S_j})$. In the case of a bad condition we discard those points that determine instability. We indicate with $Y_1^\star$ the set of the points $y_k^\star \in Y_0^\star$ not discarded.

The set $Y_1^\star$ has been determined on the basis of local interpolation matrices well conditioned, but this does not ensure that the global matrix $A_{Y_1^\star,Y_1^\star}$ is numerically stable. In fact it could happen that, when subdividing the set $Y_0^\star$ into subsets, some geometry of points of the global set have been split. When the matrix $A_{Y_1^\star,Y_1^\star}$ is unstable, the step of the subdivision is repeated on $Y_1^\star$. The recursive process gets a set of centers well separated by few iterations. Let M_F be the cardinality of $Y^\star$. As before, we improve the covering radius by considering for each point $y_j \in Y^\star$ its Voronoi cell $V_j^\star$ and we construct the set T of the barycenters of the points $\{x_k \in X \cap V_j^\star\}$, $j = 1, \dots M_F$.

The procedure here described has low computational cost because it works on sets of small sizes. The bigger cost is due to the thinning scheme described in [3] to determine the initial set Y_0 needed when $N > M_0$. Such a cost is of the order of $N \log N$. When $N \le M_0$ the procedure takes $Y_0 \equiv X$.

The procedure, here described in short, can be suitably adapted to the case of arbitrary distributions. In the already cited report [6] the cases of uniform distribution, clusters of data and distributions dependent on the phenomenon are considered.

§5. Examples

We shall show three examples relevant to three different distributions that can be met in different applicative problems. For each one of the examples quoted, we provide: the maximum error e_∞ computed on a grid 61×61, the cardinality of the set T and the value of the index of spectral condition $\mathcal{K}_2(A_{X,T})$ provided by Matlab as well as the size N of the set X. In all the examples we take the unitary square $[0, 1]^2$ as D and we take the shifts of the multiquadric with parameter $\delta = 0.35$ as basis functions. For this basis the value of M_0 is 314.

Finally the results have been compared with some known methods in the literature, in particular with techniques of knot removal to construct the set of the centers, [4], and with the approximated interpolation, [10].

The last method has a solution given by a linear combination of shifts of a RBF$-\phi$

$$P_f(x) = \sum_1^N \hat{c}_j \phi(x - x_j)$$

whose coefficients $\{\hat{c}_j\}_1^N$ solve the system

$$(A_{XX} + \lambda I)\mathbf{c} = \mathbf{f},$$

where the parameter λ is chosen in a theoretical way based on the smoothness of the unknown function f.

5.1. Example 1

Let us consider a sample of size $N = 198$ from a distribution with variable densities depending on the behaviour of Franke's function. This way of collecting the information, relevant to

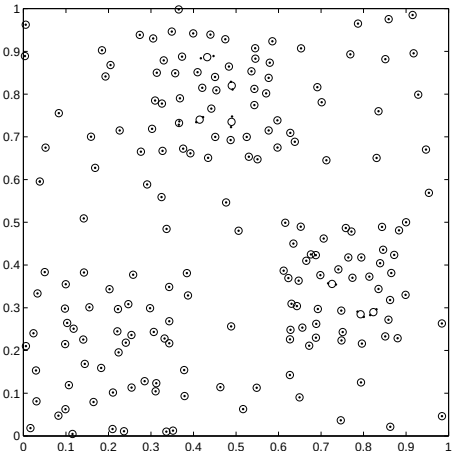

Figure 3: X dotted, T circled

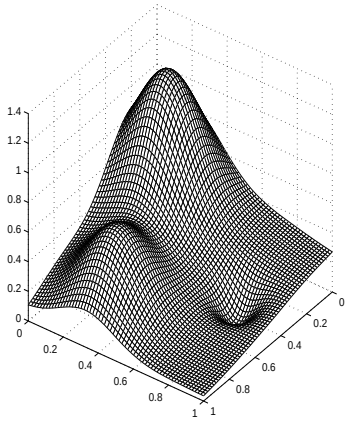

Figure 4: The approximant $s_{X,T}$

the phenomenon to be recovered at hand, is used, for example, in problems of clinical survey or in geophysical problems. In this case it is $N < M_0$ and it is $\mathcal{K}_2(A_{X,X}) = 2.38\ e(16)$ with a warning of not full rank from Matlab:

- According to the current sketched procedure the set T selected, by just one iteration, is the one shown in Fig. 3 of size 189 and with $\mathcal{K}_2(A_{X,T}) = 1.60\ e(13)$. The graphic is shown in Fig. 4 and the error is

  $$e_\infty(X, T) = 1.94\ e(-3).$$

  The running time was 0.88 sec., excluding the computation of Y_0, on a AMD 64 working as a monoprocessor.

- By using the thinning technique presented in [3] to construct the set of the centers, a set $\tilde{X}$ of 183 centers is selected.

  The set of the centers $\tilde{X}^\star$, obtained by improving the covering radius, determines a stable matrix $A_{X,\tilde{X}^\star}$ with error

  $$e_\infty(X, T) = 2.30\ e(-3),$$

  and the total running time was 1.20 sec, excluding the computation of Y_0.

- When constructing the approximated interpolation with the good value $\lambda = 10^{-10}$ we obtain

  $$e_\infty(X, X) = 2.17\ e(-3).$$

5.2. Example 2

We assign a sample of mildly scattered data of size $N = 1600$ from the valley test function, [7]. The sample is oversized to simulate the case of laser measures of a smooth feature

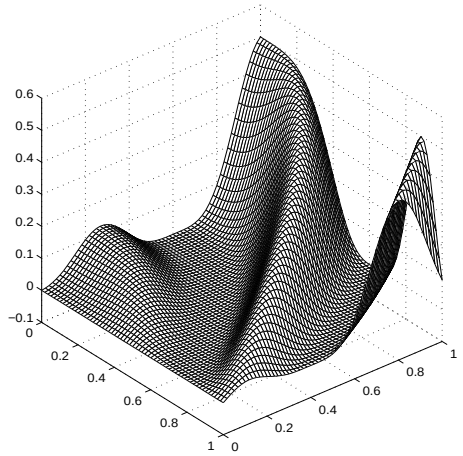

Figure 5: The approximant $s_{X,T}$

as in industrial applications. Moreover the coefficients and the centers of $s_{X,T}$ provide a compressed information for the data set.

- Our algorithm selects T of size $M = M_0 = 314$. The index of condition is $\mathcal{K}_2(A_{X,T}) = 2.92\ e(12)$ and the number of iterations is 3 . The graphical output is shown in Fig. 5 and the error is

$$e_\infty(X, T) = 1.88\ e(-3).$$

- By approximated interpolation with $\lambda = 10^{-9}$ the corresponding error is

$$e_\infty(X, X) = 8.59\ e(-3).$$

  Besides, for $N \gg M_0$, the approximated interpolation is expensive, because it is necessary to work with a full matrix $N \times N$ for each value of λ.

- By using the modified Shepard's method run with our radial basis and with the same parameters of locality as described in [5], we obtain an error

$$e_\infty(X, X) = 3.20\ e(-3).$$

  If we want a maximum error as small as the one obtained with our procedure, we have to consider a sample of size $N > 3000$.

5.3. Example 3

Here we consider the case of a configuration of clusters of points. Cluster sampling has many analogies to real-world sampling. It is a set of densely sampled areas with large gaps where no samples are taken, [8]. $N = 131$ data from Franke's test function are taken with $X = \cup_{r=1}^{n=25} S_r$ where with $\{S_r\}$ we have named the clusters, as shown in Fig. 6. The value of

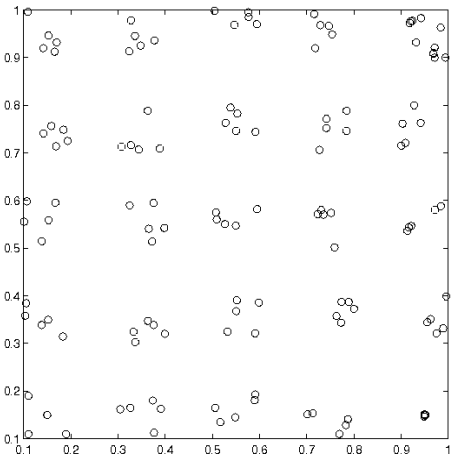

Figure 6: X locations

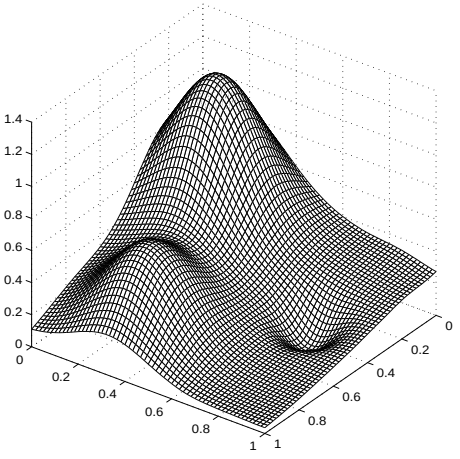

Figure 7: The approximant $s_{X,T}$

M_0 for this configuration is 260; so we put $Y_0 \equiv X$. The algorithm, working locally, by one iteration, determines the set T by discarding one point only belonging to the 25-th cluster located in the top right hand corner. It turns out that $M = 130$ and $\mathcal{K}_2(A_{X,T}) = 4.11\ e(13)$.

The graphical output of $s_{X,T}$ is shown in Fig. 7 and the error is

$$e_\infty(X, T) = 3.80\ e(-2).$$

There are cases where there are some points very near each other, as happens in the case of real-world sampling. We could use an adaptive technique that exchanges the data of locations, that are very near each other, with the average of their functional values, placed at their barycenter. By using such a technique in our case, the associated interpolation matrix $A_{\tilde{X},\tilde{X}}$ presents $\mathcal{K}_2(A_{\tilde{X},\tilde{X}}) = 4.04\ e(13)$ and the errors of the interpolant are

$$e_\infty(\tilde{X}, \tilde{X}) = 7.56\ e(-2).$$

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