On unsymmetric collocation by Radial Basis Functions

Y. C. Hon, City University of Hong Kong [1]

R. Schaback, University of Göttingen [2]

Abstract. Solving partial differential equations by collocation with radial basis functions can be efficiently done by a technique first proposed by E. Kansa in 1990. It rewrites the problem as a generalized interpolation problem, and the solution is obtained by solving a (possibly large) linear system. The method has been used successfully in a variety of applications, but a proof of nonsingularity of the linear system still was missing. This paper shows that a general proof of this fact is impossible. However, numerical evidence shows that cases of singularity are rare and have to be constructed with quite some effort.

1 Introduction

A large variety of numerical techniques can be formulated as generalized interpolation problems on spaces of multivariate functions. An easy special case is provided by **collocation methods**. These use an N-dimensional space S of functions and N functionals $\lambda_1, \ldots, \ldots\lambda_N$. The space S is spanned by functions $f_1, \ldots, f_N$, and then one looks for a function

$$f = \sum_{j=1}^{N} \alpha_j f_j \in S$$

such that the system

$$\lambda_k(f) = \sum_{j=1}^{N} \alpha_j \lambda_k(f_j),\ 1 \leq k \leq N \tag{1}$$

[1] Supported by City Univ. Strategic Research Grant No. 7000943

[2] Visiting City Univ. of Hong Kong, sponsored by DFG

is uniquely solvable for the coefficients $\alpha_1, \ldots, \alpha_N$. Note that (1) describes a plain interpolation problem, if the functionals $\lambda_1, \ldots, \ldots\lambda_N$ are point evaluations $\delta_{x_1}, \ldots, \ldots\delta_{x_N}$. This is why (1) can be viewed as a generalized interpolation problem.

This approach needs that the system (1)with the coefficient matrix

$$A := (\lambda_k(f_j))_{1\leq j,k\leq N}$$

is nonsingular. This paper concentrates on the question of singularity of such matrices in the special case of spaces spanned by radial basis functions.

In fact, radial basis functions of the form

$$\phi(\|x-y\|_2)\ x, y \in \mathbb{R}^d,\ \phi\ :\ \mathbb{R} \to \mathbb{R}_{\geq 0}$$

provide an easy and effective approach to spaces of multivariate functions. For scattered "centers" $x_1, \ldots, x_N$ one can form the space

$$S := \text{span}\,\{\phi(\|\cdot - x_j\|_2) \quad 1 \leq j \leq N\}$$

and use this space in the above setting. If the data functionals are the point evaluation functionals $\delta_{x_1}, \ldots, \ldots\delta_{x_N}$, the problem is a pure interpolation problem and the matrix A is symmetric with entries $\phi(\|x_i - x_j\|_2)$.

However, even in this simple situation it may happen that the matrix is singular. This occurs, for instance, in case of Hardy's multiquadrics $\phi(r) := \sqrt{r^2+c^2}$ and for thin–plate splines $\phi(r) := r^2 \log r$.

One has to add a space $\mathbb{P}^d_m$ of d–variate polynomials of order (=degree-1) at most m and to kill the additional $q := \dim \mathbb{P}^d_m$ degrees of freedom by the additional requirement

$$\sum_{j=1}^{N} \alpha_j p(x_j) = 0 \ \text{ for all } p \in \mathbb{P}^d_m \tag{2}$$

for the solution of the system (1). If m is chosen large enough ($m \geq 1$ for multiquadrics, $m \geq 2$ for thin–plate splines), the resulting augmented system will be nonsingular. We refer te reader to standard literature on radial basis functions for a deeper understanding of these facts.

2 Kansa's Technique

A special but important case occurs for collocation for the inhomogeneous Dirichlet problem on a bounded domain $\Omega \subset \mathbb{R}^2$, using multiquadrics. We have $m \geq 1$ and split the functionals $\lambda_1, \ldots, \lambda_N$ in two parts:

- Lagrange data functionals $\delta_{x_1}, \ldots, \delta_{x_M}$ for points on the boundary of the domain Ω,
- Laplace data functionals $\Delta_{x_{M+1}} = \delta_{x_{M+1}}\Delta, \ldots, \Delta_{x_N} = \delta_{x_N}\Delta$ for points in the closure of the domain.

Collocation is done with the span of the functions $\phi(\|\cdot - x_j\|_2)$, $1 \leq j \leq N$ plus the functions in $I\!P_m^d$. The additional condition (2) is imposed.

The method was first introduced by Ed Kansa [12, 13] and used successfully (and for more general settings) by several other authors, e.g. [1, 2, 3, 14].

Hon et al. further extended the use of the MQ-RBFs on the numerical solutions of various ordinary and partial differential equations including general initial value problems [9], nonlinear Burgers' equation with shock wave [10], surface wind field computation from scattered data [5], complicated biphasic and triphasic models of mixtures [7][8], shallow water equation for tide and currents simulation under irregular boundary [6], and free boundary problems like American option pricing [11]. The computations showed the definite advantages in using this truly mesh-free MQ-RBFs for solving various initial and boundary values problems.

The corresponding $(N+q) \times (N+q)$ matrix was always found to be nonsingular, but there was no proof of this fact. In this paper, we construct counterexamples, but the construction shows that counterexamples are rare birds indeed.

In the above technique, the functionals $\delta_{x_1}, \ldots, \delta_{x_N}$ generating the space

$$S := \text{span}\left\{\delta_{x_j}^t \phi(\|\cdot - t\|_2) \quad 1 \leq j \leq N\right\}$$

are different from the collocation functionals $\lambda_1, \ldots, \lambda_N$, making the collocation matrix unsymmetric. Here, we used the superscript t to denote action of a functional with respect to the variable t. If one uses the collocation functionals $\lambda_1, \ldots, \lambda_N$ to generate the space

$$S := \text{span}\left\{\lambda_j^t \phi(\|\cdot - t\|_2) \quad 1 \leq j \leq N\right\},$$

a symmetric collocation technique first proposed by Wu [16] results, and under mild assumptions on ϕ and the functionals $\lambda_1, \ldots, \lambda_N$ the symmetric collocation matrix with entries $\lambda_j^s \lambda_k^t \phi(\|s - t\|_2)$ is positive definite. However, symmetric collocation needs stronger regularity assumptions and usually provides inferior numerical results (see e.g. Fasshauer [4]). This is why Kansa's unsymmetric collocation is to be preferred.

3 Theoretical Basis for Counterexamples

To be not too far away from any application, we took the Poisson equation on the square $\Omega = [-1,+1]^2$ and fixed $M = 8$ Lagrange data points equidistantly on the boundary (corners and mid–edges). Another 9 points for collocation of Laplacian values were placed inside the square, and we vary these 9 points later. Since applications have concentrated on multiquadrics, these were used here, too. Since they require $m = 1$, we added a constant function and a single additional condition (2) on the coefficients of the actual 17 radial basis functions. This is the minimum requirement to make the pure interpolation problem nonsingular. Altogether, we thus have an 18×18 matrix $A(Y)$, whose entries are smooth functions of the elements of the Laplacian center set $Y = \{x_9, \ldots, x_{17}\} \subset [-1,+1]^{18}$.

We carried out similar calculations for other radial basis functions, and therefore we describe the technique in somewhat more general terms. However, we used the same geometric setting in all cases. The determinant $D(Y) := \det A(Y)$ is a smooth function on $[-1,+1]^{18}$, and for a counterexample it suffices to find two numerically nondegenerate cases $Y_1,\ Y_2 \in [-1,+1]^{18}$ with $D(Y_1) \cdot D(Y_2) < 0$. We can then conclude that on any continuous path in $[-1,+1]^{18}$, joining Y_1 and Y_2, the determinant must vanish at least once. But there are lots of such paths that avoid coalescing points, and each path gives at least one counterexample with noncoalescing points and zero determinant.

To find two numerically nondegenerate cases $Y_1,\ Y_2 \in [-1,+1]^{18}$ with $D(Y_1) \cdot D(Y_2) < 0$, we ran a large number of evaluations of $D(Y)$, each with a random choice of Y. It turns out that sign changes of the determinant are very rare, and one just has to look for a single case with the "wrong" sign of the determinant. We discarded examples where two of the 9 randomly chosen points with Laplacian data had a distance less than 0.1, because there are trivial zeros of the determinant whenever two points coalesce, and we do not want cases with very small determinants in absolute value. Cases with a large condition number in relation to the absolute value of the determinant were discarded, too, because they do not provide safe examples. More precisely, we insisted on the condition

$$\mathrm{cond}\,(A(Y))/|\det(A(Y))| < 10^{10}$$

when doing everything in 64–bit double precision. However, it suffices to verify a posteriori that the final exceptional example really has the "wrong" sign of determinant, even with roundoff taken into consideration.

4 Numerical Results

After 7846 samples for multiquadrics with $c = 0.5$ we found an exceptional configuration with the following Laplace points:

8.273563011676801e-01	1.802418079135202e-01
2.394614691098507e-01	-3.252848579200380e-01
9.794477615409753e-01	-9.277954753152073e-01
-9.372443072205616e-01	-2.431062149084667e-01
8.888265033666167e-01	-5.002654378769293e-01
1.633663452991128e-01	4.030965172700103e-01
-9.984683087088486e-01	5.822021935983579e-02
-7.520452098697639e-02	-3.715893613973583e-01
3.489601022326201e-01	1.330205365703536e-01

A plot of these points is in Figure 1. This case has determinant -1.265 and condition 23764.4, while the preceding sample (for instance) had determinant 46.2. To make sure that there is no serious loss of accuracy, we calculated the approximate inverse of $A(Y)$ and found the norm of the residual to be 6.5e-13. Further evidence was provided by looking at the full Gaussian elimination process: the pivots were reasonable in all elimination steps. By our continuity argument, this example shows that a general proof of nonsingularity of the unsymmetric collcation matrix is impossible.

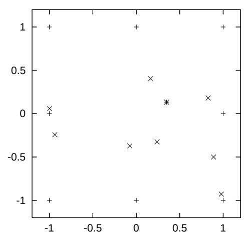

Figure 1: Points leading to “wrong” sign of determinant. Here, the + marks stand for the Lagrange points on the boundary, the x marks are the random Laplace collocation points in the interior, while the * mark is the Laplace collocation point that we later moved around to produce the plot of the determinant following in the next figure.

If the most central point y is moved around, the determinant $d(y) := D(Y(y))$ produces a function on $[-1,+1]^2$, plotted in Figure 2.

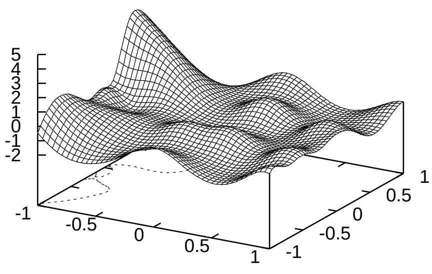

Figure 2: Determinant as function of single point

There is a well–defined zero contour line, and by a sequence of numerical examples (minimization of the absolute value of the determinant on locally refined grids) we finally got a strongly degenerate case with a determinant of 8.212515803804915e-11, where the *–marked point of Figure 1 has moved to the place $(x, y) = (\texttt{-4.500777547787466e-01,5.271590048254461e-01})$ in Figure 3.

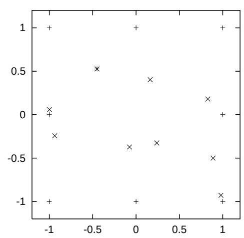

Figure 3: Degenerate points

The points are still well–separated, but the condition 6.04e+14 is extremely bad and the determinant -8.4e-11 is extremely small. However, the row–sum norm of the residual matrix still is 1.425951247620105e-02, proving that this case is at the very edge of computability with 64 bit double precision floating point numbers.

In case of polynomial degree 1 we have to work wit a 20×20 matrix. It now takes 292372 samples to get a determinant of -0.125 against 1723.0 in the previous sample, and with condition 2.18e+5. The points are in Figure 4, and the corresponding determinant plot is Figure 5.

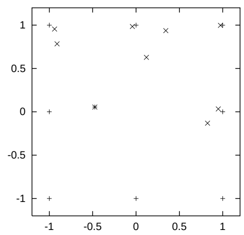

Figure 4: Multiquadrics counterexample with linear polynomials added

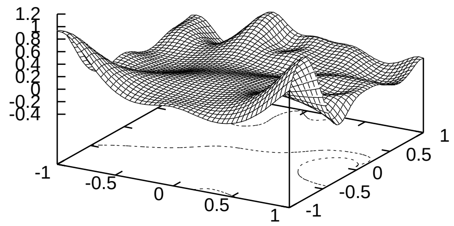

Figure 5: Determinant plot of multiquadrics counterexample with linear polynomials added

The technique also works for Gaussians with no polynomials added, and it took just 390 samples. The matrices now are 17×17. The points of the case with "wrong" sign of determinant are in Figure 6, and the corresponding determinant plot is Figure 7.

We carried out many test runs with Wendland's C^2 function $\phi(r) = (1-r)_+^4(1+4r)$ at various scales (i.e. using $\phi(r/c)$ for different c to have support radius c).

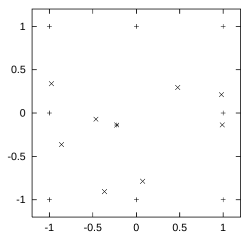

Figure 6: Gaussian counterexample

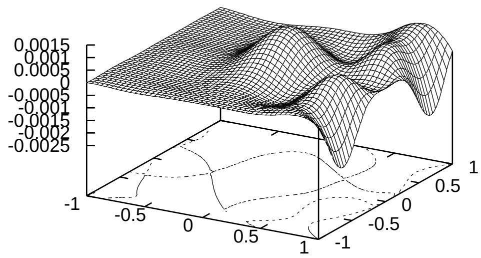

Figure 7: Determinant plot of Gaussian counterexample

For sufficiently small c in relation to the minimal distance of data points, these functions will generate diagonal collocation matrices with nonzero entries on the diagonal. But these nondegenerate cases have large discretization errors and are thus practically useless. For this reason we tested cases with large c only, but no counterexamples were found so far. However, we do not believe that these compactly supported radial basis functions from [15] always generate nonsingular matrices.

5 Conclusion

We have shown that there cannot be a general proof of nonsingularity of matrices arising from unsymmetric collocation with radial basis functions. Since nonsingularity was observed in all practically relevant cases, theoretical investigations can now proceed to prove nonsingularity in restricted situations.

For applications, unsymmetric collocation still is preferable over symmetric collocation due to its superior performance. The pure existence of singular cases is no serious objection to a valuable numerical technique. For example, numerical analysts still solve linear systems of equations even though they can be singular in certain cases. There are reliable techniques to detect near–singularity of matrices, and if these techniques are incorporated into running code, applications are safeguarded.

References

[1] Dubal, M.R., Construction of three-dimensional black-hole initial data via multiquadrics, Phys. REv. D. **45** (1992), 1178–1187.

[2] Dubal, M.R., Domain decomposition and local refinement for multiquadric approximations. I: Second-order equations in one-dimension, J. Appl. Sci. Comp. **1** (1994), 146-171.

[3] Golberg, M.A. and C.S. Chen, Improved multiquadric approximation for partial differential equations, Engr. Anal. with Bound. Elem. **18** (1996), 9–17.

[4] Fasshauer, G., Solving partial differential equations by collocation with radial basis functions, in: *Surface Fitting and Multiresolution Methods*, A. LeMéhauté, C. Rabut, and L.L Schumaker, eds., Vanderbilt University Press, Nashville, 1997, 131–138.

[5] Hickernell, F.J. and Y.C. Hon, Radial basis function approximation of the surface wind field from scattered data, Appl. Sci. Comput. **4** (1998), 221–247.

[6] Hon, Y.C., K.F. Cheung, X.Z. Mao, and E.J. Kansa, A multiquadric solution for shallow water equation, ASCE Journal of Hydraulic Engineering, May 1999, to appear.

[7] Hon, Y.C., M.W. Lu, W.M. Xue, and Y.M. Zhu, Multiquadric method for the numerical solution of a biphasic model, Appl. Math. Comput. **88** (1997), 153–175.

[8] Hon, Y.C., M.W. Lu, W.M. Xue, and X. Zhou, A new formulation and computation of the triphasic model for mechano-electrochemical mixtures, to appear at the Journal of Computational Mechanics, 1999.

[9] Hon, Y.C. and X.Z. Mao, A multiquadric interpolation method for solving initial value problems, Sci. Comput. **12/1** (1997), 51–55.

[10] Hon, Y.C. and X.Z.Mao, An efficient numerical scheme for Burgers' equation, Appl. Math. Comput. **95** (1988), 37–50.

[11] Hon, Y.C. and X.Z. Mao, A radial basis function method for solving options pricing models, Journal of Financial Engineering, March 1999, to appear.

[12] Kansa, E.J., Multiquadrics-a scattered data approximation scheme with applications to computational fluid dynamics-I. Surface approximations and partial derivative estimates, Comput. Math. Applic. **19** (1990), 127–145.

[13] Kansa, E.J., Multiquadrics-a scattered data approximation scheme with applications to computational fluid dynamics-II. Solutions to hyperbolic, parabolic, and elliptic partial differential equations, Comput. Math. Applic. **19** (1990), 147–161.

[14] Kansa, E.J., A strictly conservative spatial approximation scheme for the governing engineering and physics equations over irregular regions and inhomogeneous scattered nodes, Comput. Math. Applic. **24** (1992), 169-190.

[15] Wendland, H., Piecewise polynomial, positive definite and compactly supported radial basis functions of minimal degree, Adv. Comput. Math. **4** (1995), 389–396.

[16] Wu, Z., Hermite-Birkhoff interpolation of scattered data by radial basis functions, Aprox. Theory Appl. **8** (1992), 1–10.