Unisolvence of randomized MultiQuadric Kansa collocation for convection-diffusion with mixed boundary conditions

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Abstract

We make a further step in the open problem of unisolvence for unsymmetric Kansa collocation, proving that the MultiQuadric Kansa method with fixed collocation points and random fictitious centers is almost surely unisolvent, for stationary convection-diffusion equations with mixed boundary conditions on general domains. For the purpose of illustration, the method is applied in 2D with fictitious centers that are local random perturbations of predetermined collocation points.

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1. Introduction

In the recent paper [15] a further step has been made in the open problem of unisolvence for unsymmetric Kansa collocation, proving that collocation matrices for elliptic equations by Polyharmonic Splines (without polynomial addition) with fixed collocation points and random fictitious centers are almost surely invertible. Domains and boundary conditions are general (mixed type). The proving technique (by induction on determinants) is based on the fact that Polyharmonic Splines are real analytic but have a singularity at the center, that can be exploited to prove the key property of linear independence of the functions involved in collocation.

In the present note we extend such unisolvence result to the case of Kansa collocation by Multiquadrics, widely studied and applied after the pioneering work of E.J. Kansa [8, 9]; cf. e.g. [4, 6, 13, 18] with the references therein. The proof is more difficult with respect to Polyharmonic Splines, since MultiQuadrics are everywhere analytic so real singularities cannot be exploited to prove linear independence of the involved functions. Indeed, we have to resort to a complex embedding in order to to exploit the presence of complex singularities.

We prove the result for stationary convection-diffusion equations on general domains with mixed Dirichlet-Neumann boundary conditions. A key aspect is that the centers are kept distinct from the collocation points and randomly chosen, so that the framework is different from [1, 5] where the classical (but tricky) case of random collocation points coinciding with the centers was considered, for the Poisson equation with purely Dirichlet boundary conditions. Indeed, the present framework allows to include in a simple way the Neumann conditions.

Moreover, the fictitious centers are any continuous random vector, so that in practice they can be chosen as local random perturbations of both the interior and the boundary fixed collocation points, ensuring in any case almost sure unisolvence of the collocation process. The collocation points can be taken deterministically, for example with a uniform or quasi-uniform distribution in the interior and on the boundary of the domain. Determining sufficient conditions for unisolvence is relevant, since it is well-known after Hon and Schaback

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[7] that it could not hold in the purely deterministic case, but there is still a substantial lack of theoretical results on this subject.

The paper is organized as follows. In Section 2 we give the main theoretical result, based on a quite general lemma on unisolvence of interpolation in analytic function spaces. In Section 3 we present a couple of numerical examples, showing the practical applicability of randomized Kansa collocation with fictitious centers, chosen as local random perturbations of predetermined collocation points.

2. Unisolvence of MQ Kansa collocation

We consider stationary convection-diffusion equations with constants coefficients and mixed boundary conditions

$$\begin{cases} \mathcal{L}u(P) = \Delta u(P) + \langle \nabla u(P), \vec{v}(P) \rangle = f(P) \ , \ P \in \Omega \subset \mathbb{R}^d \ , \\ \\ \mathcal{B}u(P) = \chi_{\Gamma_1}(P)u(P) + \chi_{\Gamma_2}(P)\partial_\nu u(P) = g(P) \ , \ P \in \partial\Omega \ , \end{cases} \tag{1}$$

where Ω is a bounded domain (connected open set), $P = (x_1, \dots, x_d)$, $\Delta = \partial^2_{x_1} + \cdots + \partial^2_{x_d}$ is the Laplacian, $\nabla = (\partial_{x_1}, \dots, \partial_{x_d})$ denotes the gradient, $\vec{v}(P)$ a velocity field and $\langle \cdot, \cdot \rangle$ the inner product in $\mathbb{R}^d$, $\partial_\nu = \langle \nabla, \vec{\nu} \rangle$ is the normal derivative at a boundary point, and χ denotes the indicator function. The boundary is indeed splitted in two disjoint portions, namely $\partial\Omega = \Gamma_1 \cup \Gamma_2$, and $g(P) = \chi_{\Gamma_1}(P)g_1(P) + \chi_{\Gamma_2}(P)g_2(P)$, where g_1 and g_2 are given functions defined on those portions of the boundary. If $\Gamma_2 = \emptyset$ or $\Gamma_1 = \emptyset$ we recover purely Dirichlet or purely Neumann conditions, respectively. Observe that for notational simplicity we have taken the diffusion coefficient equal to 1, with no loss of generality since otherwise we can absorb it in $\vec{v}$ and f. As known, equation (1) models the steady state of convection-diffusion with an incompressible flow. We do not make here any restrictive assumption on the domain Ω and on the functions $\vec{v}$, f and g, except for those ensuring well-posedness and sufficient regularity of the solution (for example that the domain has a Lipschitz boundary, cf. e.g. [17] with the references therein).

We study the discretization of the convection-diffusion problem above by unsymmetric Kansa collocation using MQ (MultiQuadric) RBF (Radial Basis Functions) of the form $\{\phi_{C_j}(P)\}$, $1 \leq j \leq N$,

$$\phi_C(P) = \phi(\|P - C\|) \ , \ \ \phi(r) = \sqrt{1 + (\varepsilon r)^2} \ , \ r \geq 0 \ , \tag{2}$$

where $C = (c_1, \dots, c_d)$ is the RBF center and $\| \cdot \|$ the Euclidean norm. As known, the so-called "shape parameter" $\varepsilon > 0$ can be used to control the trade-off between conditioning and accuracy; cf. e.g. [4, 6, 12] with the references therein.

The collocation points will be fixed, whereas the centers will be chosen as a random vector. The approach where centers are distinct from the collocation points is known as collocation by "fictitious centers" in the literature, differently from the classical method, originally proposed in the pioneering work by E.J. Kansa [8, 9], where centers and collocation points coincide. Methods based on fictitious centers are an active research subfield in the literature on Kansa collocation (essentially in the least squares framework), cf. e.g. [2, 3, 20]. The possibility of taking separate collocation and center points allows more flexibility, both from the theoretical as well as the computational point of view. In particular, we will be able to prove almost sure unisolvence of the discretized problem.

Seeking a solution of the form $u_N(P) = \sum_{j=1}^N a_j \phi_{C_j}(P)$ we get the linear system

$$K_N \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix} = \begin{pmatrix} (f(P_i))_i \\ \\ (g(P_k))_k \end{pmatrix} \ , \ \ K_N = \begin{bmatrix} \mathcal{L}\phi_{C_j}(P_i) \\ \\ \mathcal{B}\phi_{C_j}(P_k) \end{bmatrix} \in \mathbb{R}^{N \times N} \ , \tag{3}$$

where $1 \leq i \leq N_I$, $N_I + 1 \leq k \leq N$, $1 \leq j \leq N$, $C_1, \dots, C_N$ are the centers, $\{P_1, \dots, P_{N_I}\} \subset \Omega$ are N_I distinct internal collocation points, and $\{P_{N_I+1}, \dots, P_N\} \subset \partial\Omega$ are $N_B = N - N_I$ distinct boundary collocation points.

Observe that taking the partial derivatives with respect to the $P = (x_1, \dots, x_d)$ variables, we easily get (cf. e.g. [6])

$$\nabla\phi_C(P) = (P - C)\,\frac{\phi'(r)}{r}\;,\;\;\Delta\phi_C(P) = \phi''(r) + (d-1)\,\frac{\phi'(r)}{r}\;,\;\;r = \|P - C\|\;, \tag{4}$$

so that

$$\mathcal{L}\phi_C(P) = \phi''(r) + (d - 1 + \langle P - C, \vec{v}(P)\rangle)\,\frac{\phi'(r)}{r}\;,\;\;P \in \Omega\;, \tag{5}$$

$$\mathcal{B}\phi_C(P) = \chi_{\Gamma_1}(P)\phi(r) + \chi_{\Gamma_2}(P)\langle P - C, \vec{\nu}(P)\rangle\,\frac{\phi'(r)}{r}\;,\;\;P \in \partial\Omega\;. \tag{6}$$

In the particular case of MQ we have

$$\frac{\phi'(r)}{r} = \varepsilon^2(1 + (\varepsilon r)^2)^{-1/2}\;,\;\;\phi''(r) = -\varepsilon^4 r^2(1 + (\varepsilon r)^2)^{-3/2} + \varepsilon^2(1 + (\varepsilon r)^2)^{-1/2}\;. \tag{7}$$

We prove now a preliminary lemma on interpolation by analytic functions, that will be relevant below.

Lemma 2.1. *Let $A \subseteq \mathbb{R}^d$, be an open connected set and $\{f_j\}_{1\le j\le N}$ be linearly independent real analytic functions in A.*

Then the set of non-unisolvent N-uples for interpolation in span$\{f_1, \dots, f_N\}$ has null Lebesgue measure in A^N.

Proof. Consider determinant of the interpolation matrix

$$D(P_1, \dots, P_N) = \det\left([f_j(P_i)]_{1\le i,j\le N}\right)\;,$$

as a function of $(P_1, \dots, P_N) \in A^N$. Such a function is analytic in A^N since analytic functions form an algebra. Notice that A^N is open and connected, being a product of open connected sets (cf. e.g. [16]). By a known general result on interpolation by linearly independent continuous functions (cf. [13]), there exist N-uples in A^N such that $D(P_1, \dots, P_N)$ does not vanish. Hence D is not identically zero in A^N. In view of a fundamental theorem in the theory of real analytic functions (cf. e.g. [14]), then the zero set of D in the open connected set A^N has null Lebesgue measure. □

We are now ready to state and prove the following

Theorem 2.1. *Let K_N be the MQ Kansa collocation matrix in (3) for the convection-diffusion problem (1), where $\{P_i\,,\,1 \le i \le N_I\} \subset \Omega$ and $\{P_k\,,\,N_I + 1 \le k \le N\} \subset \partial\Omega$ are any two fixed sets of distinct internal and boundary collocation points, respectively, and $X = (C_1, \dots, C_N)$ a continuous random vector with probability density $\sigma(X) \in L^1_+(\mathbb{R}^{dN})$.*

Then the matrix K_N is almost surely nonsingular.

Proof. The key observation is that, once fixed the set of distinct collocation points $\{P_i\}$, the matrix K_N can be seen as the transpose of the interpolation matrix at the points $C_1, \dots, C_N$, with the functions

$$f_1(C) = \mathcal{L}\phi_C(P_1), \dots, f_{N_I}(C) = \mathcal{L}\phi_C(P_{N_I}),$$

$$f_{N_I+1}(C) = \mathcal{B}\phi_C(P_{N_I+1}), \dots, f_N(C) = \mathcal{B}\phi_C(P_N)\;. \tag{8}$$

Such functions are real analytic in $A = \mathbb{R}^{dN}$, in view of (4)-(7) and the analyticity in $r \in \mathbb{R}$ of the univariate function $(1 + (\varepsilon r)^2)^s$, $s \in \mathbb{R}$. In order to apply Lemma 2.1, we have to prove that the functions $f_1(C), \dots, f_N(C)$ are linear independent.

Now, assume that they were dependent. Then, there is an everywhere vanishing linear combination, $F(C) = \sum_{j=1}^{N} \alpha_j f_j(C) \equiv 0$, with $\alpha_\ell \ne 0$ for some ℓ. Take the line $C(t) = P_\ell + tU$ with any fixed unit vector $U = (u_1, \dots, u_d)$, then the univariate analytic function $F(C(t))$ is identically zero in $\mathbb{R}$ and thus its complex extension $F(C(z))$ is identically zero in $\mathbb{C}$. Notice that the functions $(1+\varepsilon^2\|P_j - C(z)\|)^s = (1+\varepsilon^2\|P_j - P_\ell - zU\|^2)^s$ for $s = 1/2, -1/2, -3/2$, appearing in the complex extension of the functions $f_j(C(z))$, correspond to the branch of the fractional powers which is positive on the real positive axis. Moreover, $\|P_j - P_\ell - zU\|^2$ has to be seen as the complex extension of the corresponding real function, hence not the complex 2-norm but the sum of the squares of the complex components.

Then $(1+\varepsilon^2\|P_\ell - C(z)\|^2)^s = (1+\varepsilon^2 z^2)^s$ presents two branching points at $z = \pm i/\varepsilon$, whereas for $j \neq \ell$ the functions $(1+\varepsilon^2\|P_j - P_\ell - zU\|^2)^s$ are analytic at $z = \pm i/\varepsilon$, since the complex numbers

$$1+\varepsilon^2\|P_j - P_\ell - (\pm i/\varepsilon)U\|^2 = 1+\varepsilon^2\sum_{h=1}^{d}(P_j - P_\ell \mp iU/\varepsilon)_h^2$$

$$= 1+\varepsilon^2\sum_{h=1}^{d}[(P_j - P_\ell)_h^2 \mp 2i(P_j - P_\ell)_h u_h/\varepsilon - u_h^2/\varepsilon^2]$$

$$= \varepsilon^2\sum_{h=1}^{d}(P_j - P_\ell)_h^2 \mp 2i\varepsilon\sum_{h=1}^{d}(P_j - P_\ell)_h u_h$$

have positive real part. But $F(C(z)) \equiv 0$ means that $f_\ell(C(z))$ is a linear combination of the functions $f_j(C(z))$, $j \neq \ell$, and this gives immediately a contradiction, since the latter are analytic at the branching points present in $f_\ell(C(z))$ by (5)-(7).

At this point we can apply Lemma 2.1, obtaining that the set of N-uples of centers $X = (C_1, \ldots, C_N)$ for which the collocation matrix K_N is singular, has null Lebesgue measure in $\mathbb{R}^{dN}$. Consequently, it has null measure with respect to any absolutely continuous measure with respect to the Lebesgue measure, and hence the matrix K_N is almost surely nonsingular for any distribution of centers by a continuous probability measure with density $\sigma(X) \in L_+^1(\mathbb{R}^{dN})$. □

Remark 2.1. *It is worth observing that the possible center distribution is more general than that assumed in [15], where the fictitious centers are a sequence of i.i.d. (indipendent identically distributed) random points. Indeed in the present framework the multivariate probability density may not even be a product density.*

3. Numerical examples

Though the main purpose of the present work is theoretical, making a further step within the theoretical open problem of Kansa collocation unisolvence, the method of random fictitious centers can be conveniently adopted with suitable cautions and tricks. Indeed, while the random center distribution in Theorem 2.1 is quite general and the random centers could be placed in principle anywhere, still ensuring almost sure unisolvence, in practice the method works much better with centers located near the collocation points. On the other hand, it is well-known that the MQ collocation matrices can be severely ill-conditioned and a specialized literature exists on different approaches to cope with ill-conditioning, such as for example shape parameter optimization, extended precision arithmetic, RBF-QR method; cf., e.g., [6, 10, 11, 12] with the references therein.

For the mere purpose of illustration we present some simple numerical examples, concerning the solution of convection-diffusion equations with mixed boundary conditions on a square, by randomized Kansa collocation with MultiQuadrics, implemented in Matlab. We consider the convection-diffusion problem (1) on $\Omega = (0,1)^2$. In all the test problems, the set of fixed collocation points $\mathcal{C} = \{P_j\}_{1\le j\le N}$ is a uniform grid on the square, in lexicographic order. Using a Matlab notation, the random fictitious centers

$$X = \mathcal{C} + (2 * \mathrm{rand}(N,1) - 1) * \delta$$

are obtained by local random perturbation of the collocation points via additive uniformly distributed random points in $(-\delta,\delta)^2$; see Fig. 1. The accuracy is measured by the geometric mean of Root Mean Square Errors $\mathrm{RMSE}_{av} = \exp\left(\frac{1}{m}\sum_{l=1}^{m}\log_{10}\left(\sqrt{\sum_j (u_j - \tilde{u}_{j,l})^2/N}\right)\right)$ obtained by m random centers arrays

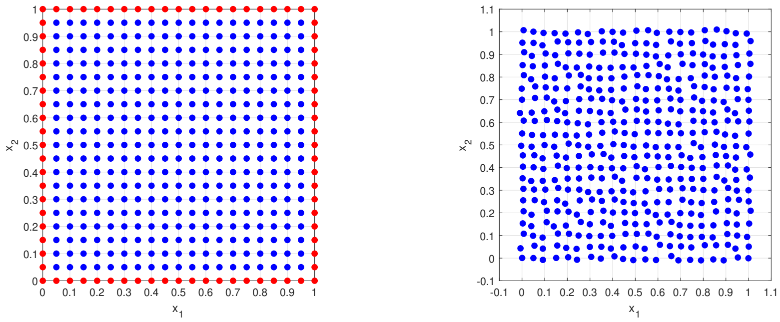

Figure 1: 441 collocation grid points (left) and the random fictitious centers distribution (right) for $\delta = 0.01$.

Table 1: RMSE geometric mean over 100 trials of N random fictitious centers, with different convection velocities $\vec{v}$ and perturbation radius δ (shape parameter $\varepsilon = 2.5$).

	$\vec{v} = (0, 0)$				$\vec{v} = (1, 1)$			
N	$\delta = 0.1$	$\delta = 0.01$	$\delta = 0.001$	$\delta = 0$	$\delta = 0.1$	$\delta = 0.01$	$\delta = 0.001$	$\delta = 0$
121	2.9e-01	6.9e-02	6.8e-02	6.9e-02	3.4e-01	7.1e-02	7.3e-02	7.2e-02
441	4.7e-02	7.9e-03	1.8e-03	1.4e-03	6.2e-02	8.2e-03	1.7e-03	1.5e-03
961	1.4e-03	9.6e-04	4.5e-04	3.4e-05	1.7e-03	9.1e-04	4.5e-04	3.5e-05
1681	4.3e-05	9.8e-06	1.0e-05	7.5e-06	4.7e-05	1.2e-05	1.2e-05	6.3e-06
	$\vec{v} = (1, 100)$				$\vec{v} = (100, 100)$			
N	$\delta = 0.1$	$\delta = 0.01$	$\delta = 0.001$	$\delta = 0$	$\delta = 0.1$	$\delta = 0.01$	$\delta = 0.001$	$\delta = 0$
121	6.1e+00	5.1e+00	3.1e+00	3.1e+00	1.6e-01	8.3e-02	4.7e-01	3.9e-01
441	2.4e+00	6.5e-01	1.1e-01	6.5e-02	1.4e-02	5.9e-03	3.7e-03	4.2e-03
961	7.7e-02	3.7e-02	2.4e-02	1.5e-03	8.5e-04	4.9e-04	2.5e-04	1.2e-04
1681	3.1e-03	8.1e-04	7.9e-04	2.1e-04	4.8e-05	2.3e-05	1.8e-05	1.9e-05

$\{X_l\}$, $l = 1, \ldots, m$, where u_j and $\tilde{u}_{j,l}$ are the exact and approximate solutions at the collocation node P_j, respectively. In the tests, we have run $m = 100$ trials.

We have imposed mixed-type boundary conditions in (1), by the splitting

$$\Gamma_1 = \{x_1 = 0,\ 0 \leq x_2 \leq 1\} \cup \{x_1 = 1,\ 0 \leq x_2 \leq 1\}\ ,$$

$$\Gamma_2 = \{x_2 = 0,\ 0 < x_1 < 1\} \cup \{x_2 = 1,\ 0 < x_1 < 1\}\ .$$

The right-hand sides f and g are defined by selecting as reference solution $u(x_1, x_2) = \sin(2\pi x_1) + \cos(2\pi x_2)$.

The numerical results are collected in Table 1, where we have taken different values of δ and different convection velocities, which make the problem ranging from pure diffusion to mildly convection-dominated instances, and we have found heuristically a value of the shape parameter ε, which roughly minimizes the errors. For strongly convection-dominated problems with high Péclet number, more specific discretization techniques should be adopted, that go beyond the scope of the present paper; cf. e.g. [19] with the references therein.

We can observe that for the smallest values of δ the errors approach the size of those corresponding to classical collocation with $X = \mathcal{C}$, which can be considered a limit case, whose unisolvence is however not covered by the present theory. For larger values of δ, e.g. $\delta = 0.1$, the errors are not satisfactory, which could be due to the fact that the separation distance of centers decreases as well as their fill distance increases, thus worsening both, the collocation matrix conditioning as well as the approximation power.

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