On Adaptive Unsymmetric Meshless Collocation

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Summary

Though the unsymmetric meshless collocation technique introduced by E. J. Kansa [5],[6] for solving PDE boundary value problems in strong form is very successful in engineering applications, there are no proven results about it so far. A greedy variation of this technique is provided here, allowing a fully adaptive data–dependent meshless selection of separated test and trial spaces.

Introduction

The general idea for solving PDE problems in strong or weak form by kernel–based meshless methods was outlined in [9]. It writes the PDE problem as an uncountably infinite number of simultaneous scalar equations

$$\lambda(u) = f_\lambda \in \mathbb{R}, \text{ for all } \lambda \in \Lambda. \tag{1}$$

The set Λ consists of infinitely many linear real–valued functionals λ that usually take the form of point evaluations of functions or derivatives at points inside a domain or on some boundary or interface layer. If several differential or boundary operators are involved, we simply put everything into a single set Λ of functionals of various types. We call (1) a *generalized interpolation problem*. Discretization just consists in replacing the infinite set Λ by some finite unstructured subset $\{\lambda_1, \ldots, \lambda_N\}$. The space spanned by these functionals can be called the *test space*. The *trial space* consists of a meshless space U of functions spanned by a basis $\{u_1, \ldots, u_M\}$, and then the discretized problem reads as

$$\lambda_i(u) = \sum_{j=1}^{M} \alpha_j \lambda_i(u_j) = f_{\lambda_i},\ 1 \le i \le N \ \text{ with } \ u := \sum \alpha_j u_j \in U \tag{2}$$

when written as linear equations for a function u of the trial space U.

For problems in strong formulation, the connection between test functionals and test functions is to be established differently. To get a truly meshless technique, and to allow very general problems, let $\Omega \subseteq \mathbb{R}^d$ be a domain, $\Phi : \mathbb{R}^d \quad \mathbb{R}^d \to \mathbb{R}$ be a *symmetric positive definite kernel* on $\mathbb{R}^d$ and associate to each functional λ a function $v_\lambda(x) := \lambda^y \Phi(x,y)$ where

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λ^y means action of λ with respect to the variable y. The standard trial space for Kansa's unsymmetric collocation method is the span of functions

$$u_j(x) = v_{\delta_{x_j}}(x) = \Phi(x, x_j),\ 1 \le j \le M, \tag{3}$$

for a set $X := \{x_1, \ldots, x_M\}$ $\mathbb{R}^d$ of suitably placed *trial centers* or *nodes*. Usually, these centers are irregularly placed within Ω. Since the scattered points determine the trial functions, we can call them *trial centers*. This leads to the unsymmetric collocation technique started by E. Kansa ([5],[6]) for the multiquadric kernel and used by many authors afterwards (see an overview in [2]).

The resulting unsymmetric collocation matrix has the entries $\lambda_i(u_j) = \lambda_i^y \Phi(y, x_j)$ and can be singular in exceptional cases [3]. Consequently, there are no mathematical results on this technique, though it gives very good results in plenty of applications in science and engineering. To overcome these problems partially, one has to modify the setting. We propose a greedy method that generates a sequence of nonsingular problems whose solutions hopefully converge to the true solution.

Asymptotic Nonsingularity

We assume the kernel Φ has an associated *native* [8] Hilbert space $\mathcal{N}_\Phi$ of functions on Ω, i.e. the kernel Φ acts as a reproducing kernel in $\mathcal{N}_\Phi$ [1]. Note that *conditionally positive definite* kernels like the multiquadrics can be modified [8] to turn into positive definite kernels by subtracting certain low–order polynomials. The given discretized strong collocation problem consists in finding a function in U such that the equations (2) are satisfied for a set $\Lambda := \{\lambda_1, \ldots, \lambda_N\}$ of linearly independent continuous linear functionals on U and prescribed real values $f_1, \ldots, f_N$. Usually, the functionals are of different types, e.g. for the Poisson problem they consist of function evaluations at the boundary and Laplacian evaluation in the interior of the domain. However, we keep the situation as general as possible, allowing quite arbitrary functionals. The linear system (2) then contains the (in general unsymmetric) N M matrix

$$A_{\Lambda,X} := (\lambda_i^x \Phi(x, x_j))_{1 \le i \le N,\ 1 \le j \le M},$$

where λ^x means evaluation of λ with respect to the variable x and where i is the row index.

While the original Kansa's method ($M = N$ and $X \subseteq \Omega$) cannot be proven to be failsafe in general, the following theorem [7] shows the asymptotic feasibility for a generalized variant using separated trial and test spaces.

Theorem 1 *Let a continuous symmetric positive definite kernel Φ on $\mathbb{R}^d$ with its native space $\mathcal{N}_\Phi$ be given. Furthermore, let a problem of the type* (1) *on a bounded domain Ω $\mathbb{R}^d$ be discretized by N linearly independent functionals $\lambda_1, \ldots, \lambda_N \in \mathcal{N}_\Phi^*$. If the trial functions are generated by* (3) *for a sufficiently dense subset X of points in Ω, the matrix $A_{\Lambda,X}$ with entries $\lambda_j^y \Phi(y, x_k)$ has full rank N.*

To make use of Theorem 1 in practice, one should fix the set $\Lambda := \{\lambda_1, \ldots, \lambda_N\}$ of N test functionals first and then work on a trial space U spanned via a very large set X of $M >> N$ trial centers [7]. The method should automatically pick N out of these M centers to guarantee nonsingularity of the resulting N by N collocation matrix.

Greedy Method

The previous section showed how to deal with a fixed set of test functionals by picking suitable subsets of trial centers in a meshless and data–dependent way. But in view of the infinite problem (1) one should also pick suitable *test functionals* in a meshless and data–dependent way, leaving the choice of trial centers to a later stage. We shall do this here, picking test functionals "greedily".

Given a large (possibly infinite) set $\Lambda \subseteq \mathcal{N}_\Phi{}^*$ of functionals. We want to reconstruct a function $u \in \mathcal{N}_\Phi$ from its data $\Lambda(u) = \{\lambda(u) : \lambda \in \Lambda\}$. Assume that a solution to Kansa's method for functionals $\lambda_1, \ldots, \lambda_n$ and suitably placed trial centers $X_n := \{x_1, \ldots, x_n\} \subseteq \mathbb{R}^d$ is known such that the corresponding matrix is nonsingular. We write this as the system

$$A_{\Lambda_n, X_n} \alpha^n = (\lambda_1(u), \ldots, \lambda_N(u))^T$$

and denote the solution function by s_n.

Now pick from Λ a functional λ_{n+1} such that $\lambda_{n+1}(s_n - u)$ is large in absolute value, possibly maximal among all other such functionals. If we find none with a nonzero value, we stop. Otherwise we conclude that λ_{n+1} must be linearly independent from the other functionals. Now add λ_{n+1} to the functionals considered so far, and add another point x_{n+1} which we still consider as a free variable. The determinant of $A_{\Lambda_{n+1}, X_{n+1}}$ is then a function v_{n+1} of $x = x_{n+1}$, in fact up to a sign

$$v_{n+1}(x) = \sum_{j=1}^{n+1} (-1)^j \lambda_j^y \Phi(y,x) \det(A_{\Lambda_{n+1} \setminus \{\lambda_j\}, X_n}) =: \sum_{j=1}^{n+1} \beta_j \lambda_j^y \Phi(y,x).$$

Now pick a fixed x_{n+1} in $\overline{\Omega}$ where this function is maximal in absolute value. If the function is zero everywhere, the functionals $\lambda_1, \ldots, \lambda_{n+1}$ are linearly dependent, which is impossible. Now repeat the iteration for $n+1$ instead of n.

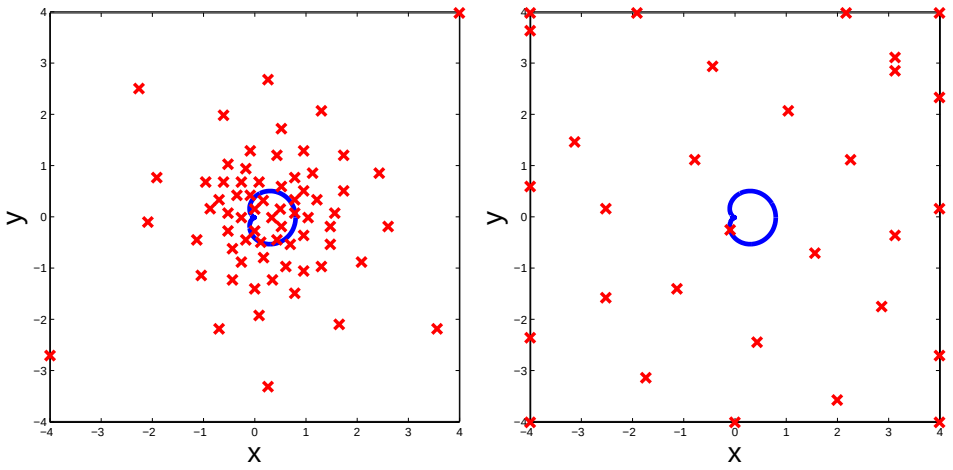
Numerical Results

Out of many possible test cases programmed in MATLAB, we take the reconstruction of a parabola at the origin from a Poisson problem with Dirichlet data on a cardioid $r = 0.4(1 + \cos\varphi)$ using the multiquadrics kernel

$$\Phi_{MQ}(y,x) := \sqrt{\|y - x\|^2 + c^2}, \quad \text{for all } x, y \in \mathbb{R}^d,$$

and various RBF-scales c. We allow the greedy method to pick from 487 test functionals and allow 8724 regularly distributed trial centers in $[-4, 4]$.

In Figure 1(a) and Figure 1(b), we graphically displayed the final trial centers distribution for RBF-scales $c = 1.25$ and $c = 6.25$, respectively. The trial centers picked by the



(a) ***Final*** 69 ***accepted centers for*** $c = 1.25$ **(b)** ***Final*** 30 ***accepted centers for*** $c = 6.25$

Figure 1: Trial centers distributions for two different RBF-scales.

greedy method lie partially outside the domain. For large RBF-scales, moreover, the greedy method prefers exterior centers. This behaviour can be observed in Figure 1 and in many other cases. Detailed results are reported below:

RBF-scale	Boundary error	Laplacian error	Solution error	CPU time	DOF
$c = 1.25$	9E-8	9E-8	4E-8	6.93 sec	69
$c = 6.25$	2E-8	3E-6	3E-8	4.23 sec	30

All root-mean-square (RMS) errors are taken as rough bounds that we suppress due to space limitations. The Dirichlet boundary residuals and the Laplace residuals inside the domain often differ in orders of magnitude, as seen in the case of $c = 6.25$. The final column denotes the actual degrees of freedom (DOF) used in the solution. Test runs also indicate that using large RBF-scales helps to save computation time, because the greedy method terminates after DOF number of iterations. The solution error for $c = 6.25$ is smaller even though its DOF is smaller. To further investigate the proposed method, Figure 2 shows the RMS errors (denoted by squares) and the degrees of freedom (denoted by circles) as a function of increasing RBF-scales. An exponential curve (denoted by a solid line) is fitted to the RMS errors. The greedy method is capable of solving problems with very large RBF-scales (up to $c = 12.5$ in this example) and is not severely influenced by the bad condition of the underlying matrix $A_{\Lambda,X}$.

In Figure 3 we present another example. The Poisson problem is solved on a smooth but irregular star-shaped domain $r = 0.3(1.5 + \cos(5\varphi))$ with Dirichlet boundary condition.

The solution is chosen to be the fundamental solution at $(2,2)$, and we use the Gaussian kernel

$$\Phi_{GA}(y,x) := \exp\left(\frac{\|y \quad x\|}{c}\right)^2, \quad \text{for all } x,y \in I\!R^d,$$

with RBF-scales that is 5 times the relative stepsize. The exponential fit reveals the convergence behaviour. As the relative step size reduces, the number of test functionals available to the greedy method increases from 51 to 2739, and the number of trial centers increases from 641 to 52719. The greedy method is capable of solving large-scale problems that cannot be handled by the original method.

Conclusion

In this preliminary form, the proposed adaptive method already demonstrates its improvement over the symmetric version [4] in terms of efficiency and accuracy. The greedy method can be run either on large discrete sets of test functionals and trial centers or on infinite sets thereof. In both cases, there is quite some chance to prove convergence to the true solution of the full problem, using the techniques of [9]. We leave this to a forthcoming paper.

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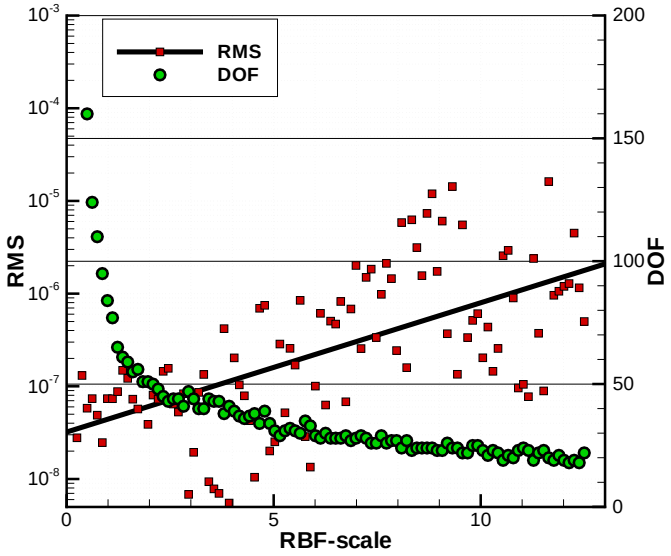

Figure 2: RMS and DOF against RBF-scale.

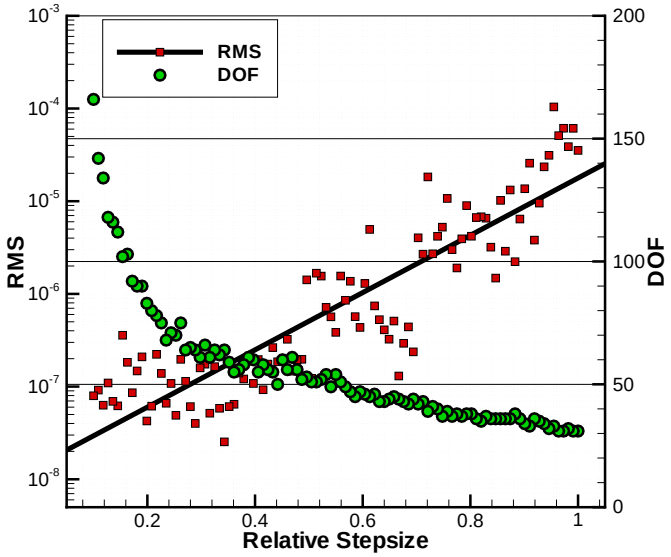

Figure 3: RMS and DOF against relative stepsize.