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Meshless Unsymmetric Collocation Method

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Summary

The history of meshless collocation methods featured plenty of nicely calculated practical solutions, but a solid mathematical basis was long missing for the most popular asymmetric technique introduced by E. Kansa. Thus the impact of this work will be to supply a lasting mathematical foundation which will also improve our general understanding of such technique. Our previous research gave a convergent algorithm.

keywords: Kansa's method, radial basis function, adaptive greedy algorithm, unsymmetric collocation

Introduction

In our previous research, we provided the first solvability and convergence results of the modified Kansa's unsymmetric collocation formulation. Readers are referred to the original articles [**?**, **?**, **?**] and an extension [**?**] to weak problems for details. As mentioned in the previous section, Kansa's original formulation may fail in certain cases even though it is widely used by many researchers. To overcome these problems partially, one has to modify the setting. To get solvability and error bounds, there should at least be a unique solution to the modified discretized system that converges to the true solution if the discretization is refined. The first question requires that if the n test functionals are fixed and are linearly independent, the system should have rank n provided the n trial centers are chosen properly. The following theorem addresses that solvability is guaranteed if the trial functions or equivalently the RBF trial centers are correctly chosen.

Theorem 1 (see [?]) *Assume the kernel Φ to be smooth enough to guarantee that the functions $u_\lambda := \lambda^y \Phi(y,\cdot)$ for $\lambda \in \Lambda$ are continuous. Furthermore, let the m functionals $\lambda_1, \ldots, \lambda_m$ of Λ_m be linearly independent over $\mathscr{U}$. Then the set of functions $\{u_\lambda\}$ for $\lambda \in \Lambda_m$ constructed above is linearly independent, and hence the unsymmetric collocation matrix is nonsingular for properly chosen trial centers.*

The theoretical part of our work showed that solvability is possible; in the practical part, the adaptive subspace selection algorithm (the so-called *greedy algorithm*) we proposed showed how it can be done efficiently in practice.

Suppose that m collocation conditions and n trial centers are provided; usually, we have $n \gg m$ to guarantee the existence of the proper subset of trial centers.

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The greedy algorithm is called *matrix–free* since the *a priori* evaluation of the full $m \times n$ matrix is unnecessary. Instead, the algorithm builds small $k \times k$ matrices starting with $k = 1, 2, 3, \ldots$ iteratively which are updated by calculations of complexity $\mathcal{O}(k^2)$ and it usually stops at rather small values of k. The termination of the algorithm depends on the computational accuracy; the selected trial centers are *chosen properly* in the sense that the resultant matrix will not crash the linear solver. If m and n are moderate in size, a QR-factorization can be employed with some trade-off of efficiency.

Our next work devoted to the convergence results of the above modified Kansa's method. Suppose the PDE is well-posed in a Hilbert space $\mathscr{U}$ with solution u^*. Let

$$\|u\|_\Lambda := \sup_{\lambda \in \Lambda} |\lambda(u)| \tag{1}$$

be a norm on $\mathscr{U}$. We would like to construct a numerical approximation $v_\varepsilon^* \in \mathscr{U}_\varepsilon$ in a finite dimensional subspace that solves the following linear optimization problem:

$$v_\varepsilon^* = \arg\min_{v \in \mathscr{U}_\varepsilon} \|v - u^*\|_\Lambda. \tag{2}$$

We can assume that, for all $\varepsilon > 0$, there is a function (e.g. the interpolant of the solution) $v_{u^*,\varepsilon} \in \mathscr{U}_\varepsilon$ with

$$\|u - v_{u^*,\varepsilon}\|_\Lambda \leq \varepsilon \|u^*\|_{\mathscr{U}}. \tag{3}$$

which is sufficient for our purpose.

Theorem 2 *[?, ?] Let $\mathscr{U}$ be a normed linear space with norm $\|.\|_{\mathscr{U}}$, dual space $\mathscr{U}^*$ and dual unit sphere $\mathscr{U}_1^* := \{\lambda \in \mathscr{U}^* : \|\lambda\|_{\mathscr{U}^*} = 1\}$. Let a test set $\Lambda \subset \mathscr{U}_1^*$ be given such that $\|.\|_\Lambda$ is defined on $\mathscr{U}$ with* (1)*. Assume further that the PDE is well-posed. Let $\{\mathscr{U}_\varepsilon\}_\varepsilon$ be a scale of subspaces of $\mathscr{U}$ for $\varepsilon \to 0$. For all $\varepsilon \to 0$, take a function v_ε^* defined by* (2)*. Then there is convergence $\|v_\varepsilon^* - u^*\|_\Lambda \to 0$.* □

Kansa–type RBF trial spaces with sufficiently dense trial centers form a sequence of subspaces getting dense in $\mathscr{U}$. We know the RBF interpolant has the required approximation power in (3) for all $\varepsilon > 0$. Hence, the convergence rate of the unsymmetric collocation method can be faster than the convergence rate of interpolation in the trial space $\mathscr{U}_\varepsilon$ with respect to the norm $\|.\|_\Lambda$ to functions in $\mathscr{U}$.

Mathematical Formulations

Our approach used a fairly recent abstract setting to be explained here. The general idea for solving PDE problems in strong or weak form by kernel–based

meshless methods is to write the problem as an uncountably infinite number of simultaneous scalar equations

$$\lambda[u] = f_\lambda \in \mathbb{R}, \quad \text{for all } \lambda \in \Lambda. \tag{4}$$

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. We call (4) a *generalized interpolation problem*.

Discretization just consists in replacing the infinite set Λ by some finite unstructured subset $\Lambda_m := \{\lambda_1, \ldots, \lambda_m\}$. The space spanned by these functionals can be called the *test space*, and Λ is the *infinite test set*.

Weak formulations use functionals of the form $\lambda_j[g] := a_j(g, u_j)$ with certain bilinear forms a_j and *test functions* u_j such that the discretized problem takes the familiar form

$$\lambda_i[u] = a_i(u, u_i) = \sum_{j=1}^{n} \alpha_j a_i(u_j, u_i) = f_{\lambda_i},\ 1 \le i \le n$$

of meshless Petrov–Galerkin schemes [**?**]. In particular, weak formulations always have a strong built–in connection of test functionals and test functions.

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, we use a symmetric positive definite kernel $\Phi : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$.

The special case of *symmetric collocation* now takes the discretized set Λ_m of test functionals and defines the trial functions as $u_j := \lambda_j^y \Phi(\cdot, y)$ for $1 \le j \le n = m$ where the superscript of λ indicates the variable of Φ on which the functional operates. Then the collocation matrix takes the symmetric form with entries $\lambda_i[u_j] = \lambda_i^x \lambda_j^y \Phi(x, y)$ for $1 \le i, j \le n$. This technique dates back to [**?**] and has a solid mathematical basis ([**?**, **?**]), as was pointed out earlier in this proposal. Like in the standard (non–Petrov) Galerkin scheme, the trial and test functions or functionals are closely related.

If one takes a set $X_n := \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$ of scattered trial centers, one can use the trial space U spanned by the trial functions

$$u_j = \Phi(\cdot, x_j),\ 1 \le j \le n$$

associated to some differential operations followed by a simple point evaluation functionals λ_{δ_j} with $\delta_j = \delta(\cdot - x_j)$. Usually, these centers are irregularly placed within Ω. This leads to the unsymmetric collocation technique started by Kansa

for the multiquadric kernel and used by many authors afterwards. The resulting unsymmetric collocation matrix has the entries

$$\lambda_i[u_j] = \lambda_i^y \Phi(y, x_j),\ 1 \le i, j \le n.$$

Consequently, there are no mathematical results on this technique, though it gives very good results in plenty of applications in science and engineering.

Lastly, our modified Kansa's method requires two set $X_n := \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$ and $Y_m := \{y_1, \ldots, y_m\} \subset \overline{\Omega}$ of scattered trial and collocation centers with $m \le n$. In practice, due to the problem of ill-conditioning, a smaller set of trial centers $X_{\hat{n}} \subset X_n$ with $\hat{n} \le m$ is selected by the greedy algorithm. If the overdetermined system

$$\lambda_i[u_j] = \lambda_i^y \Phi(y, x_j),\ 1 \le i \le m,\ 1 \le j \le \hat{n}. \tag{5}$$

is solved by linear optimization, the convergence results in Theorem 2 applies.

Discussion

Our developed error estimation is based on the infinite dimensional test space Λ. The Λ-norm (1) used in our previous work is the L^∞-norm of the PDE residual. After discretizing Λ by Λ_m, e.g. bringing the error bound from the L^∞-norm to the ℓ^∞-norm, we get a *linear optimization* (LO) problems on a discretized finite dimensional test space. In [**?**], such LO process is solved by an adaptive simplex algorithm.

The first discussion of this talk is to supply new theoretical results underpinning the meshless collocation method with easy implementation. It is well-known that the least squares optimization is numerically efficient. Since the LO is computationally much more difficult than linear system solving, this proposal focus on the convergence result when (5) is solved by least-squares (LS) optimization. In particular, we aim to prove an analog of Theorem 2 that is built upon the ℓ^2-norm of the PDE residual. The numerical part of this stage does not require any algorithm implementation; the proposed algorithm is, in fact, a (much) simpler version of our previous developed LO-based codes. For demonstration purpose, the new algorithm will be tested on some elliptic PDEs in 2D and 3D.

The result up to this point may not answer all the concerns posed by many mathematicians and engineers. It is well-known that scaling $r \leftarrow r/c$ has a strong influence to the behavior of RBF. This scaling effect is controlled by a so-called *shape parameter* c. If c is too small, the solution is usually inaccurated. On the other hand, if c is too large, the condition of the resultant matrix system becomes so bad that linear solvers may crash. Somewhere, not too small and not too large, is an optimal shape parameter that makes the RBF superior [**?**]. Thanks to a subspace selection done by the greedy algorithm, our algorithms (including both the LO-based algorithm in the previous work and the LS-based algorithm in this project)

are stable for all c. In [**?**], we demonstrated the stability of our algorithm even for some unreasonable large c. This is a relieve to the user of RBF that they should no longer worrying about picking the wrong c. However, the optimal shape parameter remains unknown. In order to generate a large trial space, that hopefully includes the one associated with the optimal shape parameter, the shape parameters will be reduced in size in successive iterations. Numerically, our proposed method can run iteratively on the PDE residual. Each iteration employs a constant shape parameter so that the error analysis in the first stage remains valid level-wise. The theory needed here is the relationship between RBF trial spaces generated by different shape parameters.

Conclusion

The future of meshless methods lies in their ability to handle problems which required complicated or time-varying discretizations. To this end, the meshless techniques themselves must be made more flexible. This is started by the practical part of this part. The pre-wavelet property of some radial basis kernels may lead to parameterfree meshless algorithms for real-life engineering problems.