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Optimality of the Method of Fundamental Solutions

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Abstract

The Effective-Condition-Number (ECN) is a sensitivity measure for a linear system; it differs from the traditional condition-number in the sense that the ECN is also right-hand side vector dependent. The first part of this work, in [EABE 33(5) pp.637–643], revealed the close connection between the ECN and the accuracy of the Method of Fundamental Solutions (MFS) for each given problem. In this paper, we show how the ECN can help achieve the problem-dependent quasi-optimal settings for MFS calculations—that is, determining the position and density of the source points. A series of examples on Dirichlet and mixed boundary conditions shows the reliability of the proposed scheme; whenever the MFS fails, the corresponding value of the ECN strongly indicates to the user to switch to other numerical methods.

1 Introduction

The Method of Fundamental Solutions (MFS) is a popular numerical method for solving homogeneous boundary value problems. For simplicity, our presentation is restricted to the homogeneous Poisson problem

$$\begin{aligned} \triangle u &= 0 \quad \text{in } \Omega \subset \mathbb{R}^2, \\ \partial_n^{(k)} u &= f_k \quad \text{on } \Gamma_k \subset \partial\Omega,\ k \in \{0,1\}, \end{aligned} \tag{1}$$

where the operator ∂_n is the outward-normal derivative, $\Gamma_0 \cup \Gamma_1 = \partial\Omega$, $\Gamma_0 \cap \Gamma_1 = \emptyset \neq \Gamma_0$, and in this paper, the functions f_0 and f_1 are called the *boundary data*

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functions which are used to generate boundary data. The MFS, belonging to a special class of Trefftz Methods [17, 18], approximates the solution of the boundary value problem (1) by linear combinations of fundamental solutions centered at source-points located outside the domain of interest. Unknown coefficients are sought to best-fit the boundary data with the singularities not ever going into the domain Ω; this is done usually by collocation but other weak-formulations work too. The applications of the MFS are very wide: from linear problems [7, 15, 31], to nonlinear equations [1, 3], and to inverse problems [4, 30]. Thorough surveys on the MFS can be found in [6, 9].

Recent research on the MFS is extensive and it is commonly believed that the MFS can always achieve highly accurate solution up to the order of machine precision. Recently, Schaback [27] made the following observation. It is usually due to convenience that many researchers choose harmonic functions to be boundary data functions for verifying the accuracy of the MFS; that is, both $\triangle f_0 = 0$ and $f_1 = \partial_n f_0$ hold in $\mathbb{R}^2$. With these *globally-harmonic* boundary data functions, the MFS calculations are always stable and its results are always accurate; both facts hold independently of the shape of Ω. Moreover, using harmonic polynomial approximations will do even better than the MFS in such situations. Many applications in engineering and science give rise to boundary data functions which are "not-that-nice." For example, the boundary control method in [23] gives subproblems with f_0 being fundamental solutions but $f_1 \equiv 0$. This either means the solution to (1) has a finite harmonic-extension outside the domain Ω or, in the serious situations, the solution or one of its derivatives has a singularity on the boundary $\partial\Omega$. All these *facts* do not make the MFS impractical, but one needs to be more cautious when employing the method. The solution provided in [27] is an adaptive algorithm that selects an appropriate basis (either a fundamental solution or a harmonic polynomial) iteratively. The algorithm there is one variation of the greedy algorithms for asymmetric meshless collocation methods [12, 14, 22, 20, 21] and it shares some common features to the matching-pursuit algorithm [25] for image processing. The full details are omitted here and we are going to present another alternative from a very different approach.

2 MFS Linear Systems and ECN

Let $\widetilde{\Omega} \supset \Omega$ be the fictitious domain. The set-up of the MFS linear system often involves placing a set of M collocation points $X = \{x_1, \ldots, x_M\}$ on the domain boundary and a set of N source points $\Xi = \{\xi_1, \ldots, \xi_N\}$ on the fictitious boundary

$\partial\widetilde{\Omega}$. The MFS approximates the solution of (1) by

$$s(x) = \alpha_0 + \sum_{j=1}^{N} \alpha_i s_j(x),\ x \in \widetilde{\Omega}. \tag{2}$$

We now have enough information to set-up an $M \times N$ linear system

$$\begin{aligned} \alpha_0 + \sum_{j=1}^{N} \alpha_j s_j(x_i) &= f_0(x_i), \quad \text{for } x_i \in \Gamma_0. \\ \sum_{j=1}^{N} \alpha_j \partial_n s_j(x_i) &= f_1(x_i), \quad \text{for } x_i \in \Gamma_1. \end{aligned} \tag{3}$$

For the Poisson problem we considered, the fundamental solution centered at the source point $\xi_j \in \Xi$ is given as

$$s_j(x) := \log \|x - \xi_j\|_2^2,$$

for $x \in \mathbb{R}^2$. Depending on the values of M and N, the linear system (3) can be a linear unsymmetric over– or underdetermined $M \times N$ system of the form $A\alpha = b$. After obtaining the unknown coefficients, the MFS approximation can be evaluated anywhere inside the fictitious domain by (2). The above procedure can be easily generalized to other types of differential equations simply by using the appropriate the fundamental solutions; see [13].

It is not difficult to see why the traditional condition number cannot be a good indicator for the MFS accuracy. The coefficient matrix A depends on the fundamental solution (i.e. the differential equation itself), and the placement of the source points and collocation points (Ξ and X); whereas the right-hand side vector $\mathbf{b}$ depends on the boundary shape, the location of the collocation points and most importantly, the boundary data functions. From [27], we know that the boundary data functions have a critical influence on to the MFS accuracy. The traditional condition number, independent of the boundary data functions, cannot provide the desired information. The *Effective-Condition-Number* (ECN), denoted by $\kappa_{\text{eff}} = \kappa_{\text{eff}}(A, b)$, is a sensitivity measure for the linear system rather than for the matrix. Namely, for $A\alpha = b$, we have

$$\frac{\|\Delta\alpha\|}{\|\alpha\|} \le \kappa_{\text{eff}} \frac{\|\Delta b\|}{\|b\|} \text{ with } \kappa_{\text{eff}} := \frac{1}{\sigma_{\min}^{+}} \frac{\|b\|}{\|\alpha\|}, \tag{4}$$

where $\sigma_{\min}^{+}$ denotes the smallest nonzero singular value of A and if A is singular, solutions to linear systems (α and $\Delta\alpha$) are obtained by the standard pseudoinverse formula.

In our first investigation [5], the following connection between the ECN and the accuracy of MFS was observed:

$$(L^{\infty} \text{ error of MFS}) \times (\text{ECN of the MFS linear system}) = \mathcal{O}(1). \tag{5}$$

The numerical experiments presented in [5], however, were rather preliminary: we did not include the constant basis in the expansion (2) and, for simplicity, we focussed on exact-determined system ($M = N$) in [5] only. We discovered later that the Accuracy-ECN relationship (5) not only holds for all situations in the MFS calculations (exact-, over-, and underdetermined) but also for a closely related method–the Boundary Knot Method [8, 29]. Readers are also referred to [16, 19] for the recent development of the MFS and ECN.

3 Optimizing the MFS Setting

Using the ECN in (4) to optimize the MFS setting has a clear advantage over using only boundary data [10]; that is, problems with Neumann or mixed boundary conditions can now be handled even though all or part of the Dirichlet data are missing. Looking for the true optimal setting for the MFS is an NP-hard (non-deterministic polynomial-time hard) problem. In some early applications of the MFS, the sources were taken to be part of the unknowns [11, 24]. More recent paper related to the optimal placement of the sources can be found in [2]. To overcome this, we have to impose some constraints. This restricts the search to a more practical way and allows us to search for a quasi-optimal setting for the MFS. First of all, the number of collocation points used, M, should be sufficiently large but fixed. The next constraint is that the fictitious boundary varies according to some predefined formulas. For example, if $\partial\Omega$ is given in polar by $r = r(\theta)$, then the fictitious domain can be constructed by $r = D + r(\theta)$ with the distance between the domain boundary and the fictitious boundary denoted by D. Users often use a circular fictitious domain with radius D regardless of the shape of Ω. In either case, the parameter D is what we try to optimize. Next, the set of N source points are distributed on the fictitious boundary according to some rules of distribution (i.e. uniformly). This allows us to search for the optimal N on a given fictitious domain.

From the Accuracy-ECN relationship (5), if we want to minimize the MFS error, the corresponding ECN should be maximized. Equivalently, we can recast the optimization problem as minimizing the inverse of the ECN. Under the imposed constraints, the N-Search and D-Search can be casted, respectively, as

$$N\text{-Search:} \quad \min_{N} \kappa_{\text{eff}}{}^{-1}\big(A, b\big), \quad \text{with } \widetilde{\Omega} \text{ fixed}, \tag{6}$$

$$D\text{-Search:} \quad \min_{D} \kappa_{\text{eff}}{}^{-1}\big(A, b\big), \quad \text{with } N \text{ fixed}. \tag{7}$$

In both searches, only one of the parameters (N and D) is treated as a scalar variable. The objective functions are scalar functions returning the ECN as output. Since the coefficient matrices are often ill-conditioned, we found that both objective functions are nonsmooth and hence (quasi-) gradient-based methods are not suitable for our optimization problems. Instead of the exhausting brute-force systematic search, we will employ the golden section search by providing lower- and upper-bounds to N and D.

Performing either one of the optimizations (6) or (7) requires fixing the other parameter *a priori*. To perform the N-Search, we need to fix a D and therefore the fictitious domain; and vice versa. To make our quasi-optimal selection closer to the real one, a sequential search can be performed. In this paper, we only consider the three-step searching processes, that is a DND-Search. With a relative small number of source points, the D-Search is faster and more importantly, experience tells us that the distance of the sources is a more important factor. It makes sense to run it twice in order to guarantee optimality. The idea of optimal setting, with no doubt, imposes a large overhead on the MFS. However, the MFS linear systems are relatively small and easy to solve. Combined with ECN, the optimized MFS becomes a more reliable subroutine for more sophisticated problems, e.g. improve the MFS subroutine in the construction of reduced basis [28].

4 Numerical Examples

To illustrate the accuracy of the proposed DND-Search procedure, we now proceed with a series of numerical demonstrations. All boundaries considered are generated by a polar function r such that $\partial\Omega = \{(r,\theta) :\ r = r(\theta),\ 0 \le \theta < 2\pi\}$. The corresponding fictitious boundary $\partial\widetilde{\Omega}$ is then constructed by $r = r(\theta) + D$ where D is the source distance to be optimized. The collocation systems are obtained using numerical expansion (2) with N (M) source points (collocation points) uniformly distributed with respect to the θ-variable on $\partial\Omega$ ($\partial\widetilde{\Omega}$). Unless otherwise mentioned, we start the first D-Search with $N = 100$ and a fixed number of collocation points $M = 400$. This means that the over-, exact-, underdetermined settings are being considered in the N-Search. The accuracy is measured either in $L^\infty(\partial\Omega)$ or $L^2(\Omega)$, respectively, for the ε_∞ and ε_2 errors; the former ε_∞ is approximated at 1000 evaluation points on the boundary and is mostly used in examples with Dirichlet boundary conditions. The latter ε_2, used in examples with mixed boundary conditions or discontinuous Dirichlet boundary conditions, is approximated with the fraction of discrete 2-norms; i.e., norm of residual in the numerator and norm of the exact function values in the denominator. The numbers of evaluation points used for approximating the $L^2(\Omega)$ errors will be reported for each care separately.

For the sake of comparison, we start by considering the examples in [27]. The

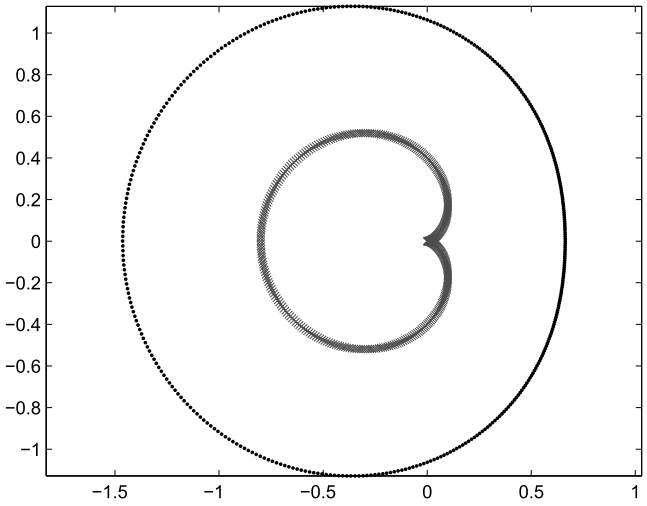

Figure 1: *MFS set-up yielded from the DND-Search for boundary data function* $f_0(x, y) = \exp(x)\cos(y)$ *on a lemniscate domain.*

first example comes with a globally-harmonic boundary Dirichlet-data function $f_0(x, y) = \exp(x)\cos(y)$ on a lemniscate domain with an incoming corner, see Figure 1. Understanding the mathematical issues suggested by Schaback, one can see that this example is trivial and highly-accurate-results are almost guaranteed independent of the MFS set-up. Our search procedure produced $\varepsilon_\infty = 5.55E-15$ using quasi-optimal parameters $D_{opt} = 0.6633$ and $N_{opt} = 400$. This yields a slightly underdetermined 400×401 system (because of the constant basis in the expansion). This is the type of *popular* test function used in many research papers– we emphasize once again that it is harder to get bad results than good ones here.

Under the same situation, the second example considers a smooth, but not harmonic, boundary data function $f_0(x, y) = x^2y^3$. With $D_{opt} = 0.8622$ and $N_{opt} = 156$, the optimized MFS yields error $\varepsilon_\infty = 4.07E-5$. The loss of ten-digits of accuracy is due to the incoming corner of the lemniscate. If the lemniscate is replaced by the unit circle, the optimal MFS yields an error $\varepsilon_\infty = 5.02E-15$ instead.

If readers compare our results in the first two examples, our proposed *DND-Search slightly* outperforms harmonic polynomials and the adaptive greedy techniques reported in [27] by one or two orders of magnitude. We now consider their last example with a non-smooth boundary data function $f_0(x, y) = \max(0, |y|)$ on the unit circle. Our search yields $D_{opt} = 0.1950$ that is much smaller than that in the previous examples. With $N_{opt} = 410$ source points, the error $\varepsilon_\infty = 1.31E-3$ is close to but not as good as the results of harmonic polynomials.

As mentioned before, the power of the proposed optimization scheme lies in the fact that it can be applied to situations in which the maximum-principle cannot

$M = 200$					
Start-N	D_{opt}	N_{opt}	ECN	ε_∞ on $\partial\Omega$	ε_2 on Ω
50	1.459E-1	202	7.28E+16	8.18E-3	8.11E-5
100	3.819E-1	346	1.09E+13	6.17E-3	6.56E-5
150	2.372E-1	198	3.76E+15	5.63E-3	5.70E-5
200	2.309E-1	200	2.41E+15	6.86E-3	6.85E-5
$M = 400$					
Start-N	D_{opt}	N_{opt}	ECN	ε_∞ on $\partial\Omega$	ε_2 on Ω
50	5.563E-2	402	9.73E+16	6.23E-3	2.95E-5
100	2.360E-1	396	1.98E+14	2.76E-3	1.69E-5
150	7.270E-2	398	6.95E+16	6.01E-3	3.04E-5
200	1.605E-1	388	3.17E+15	2.74E-3	1.69E-5

Table 1: *DND-Search results with different starting numbers of source points N.*

be applied. One such situation is for mixed boundary conditions. Consider $\Omega = [-1, 1]^2$ with Γ_1 being the top boundary and the other three being Γ_0, respectively, for imposing the Neumann and Dirichlet boundary conditions. We took $f_0(x, y) = \log((x-2)^2 + (y-2)^2)$ and $f_1(x, y) = 0$ as boundary data functions. To overcome the missing Dirichlet data on Γ_1, the problem is solved using the finite element method (FEM) with 40257 nodes at which we evaluate the $L^2(\Omega)$ error ε_2. In Table 1, we demonstrate the robustness of the DND-Search with different starting values of N and different numbers of collocation points M. A sample error distribution is also shown in Figure 2. Note also that the first D-Search is actually faster with smaller starting N. Moreover, the obtained optimal settings with different starting N are different. The quasi-optimal selections (distance D_{opt} and numbers N_{opt} of source points) vary from case-to-case. Rather than finding a fixed set-up the proposed search algorithm shows its robustness in terms of consistent accuracy. Note that the optimal number of sources tends to be very close to the number of collocation points. For efficiency, it is interesting to study if a single pass D-search on exact-determined settings is sufficient.

The last and most challenging example took the *exact solution*

$$u(x, y) = \frac{2}{\pi} \arctan \frac{2y}{1 - x^2 - y^2},$$

see Figure 3. It is a straightforward exercise to verify that u is harmonic only inside the unit circle and is discontinuous on the boundary. Readers can find more Laplace equations with singular solutions in [26].

To avoid the singularity, a scaled version of u with (x, y) replaced with $(x, y)/(1+$

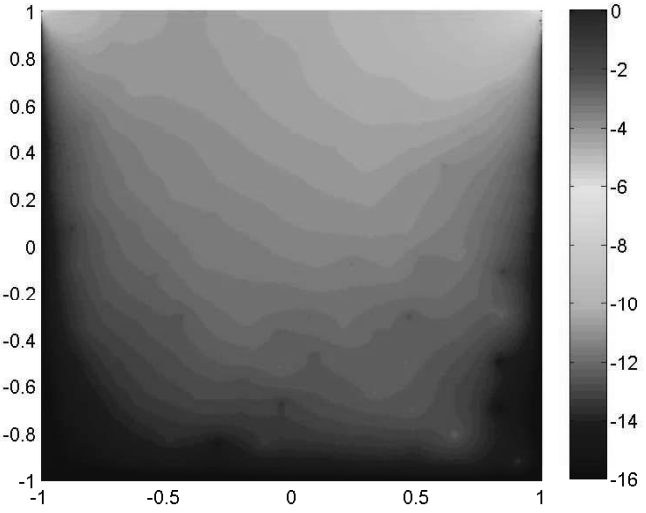

Figure 2: *Error distribution against the log-absolute error; Neumann boundary condition is imposed to the TOP boundary* Γ_1*, Dirichlet to the rest.*

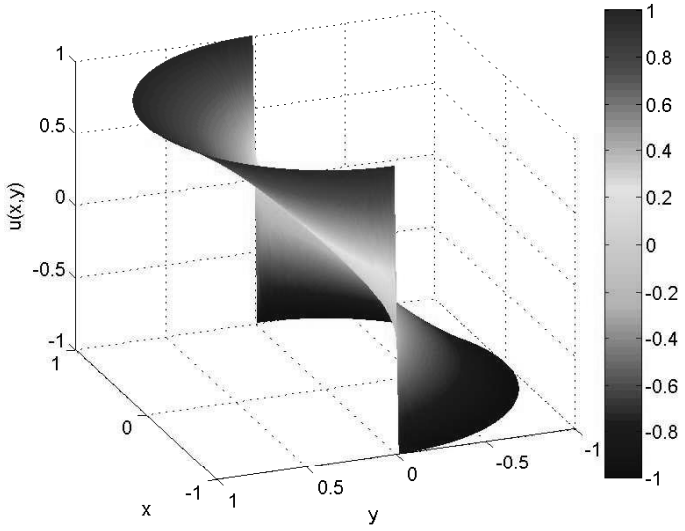

Figure 3: *Plot of* $u(x,y) = \frac{2}{\pi} \arctan \frac{2y}{1-x^2-y^2}$ *on the unit circle.*

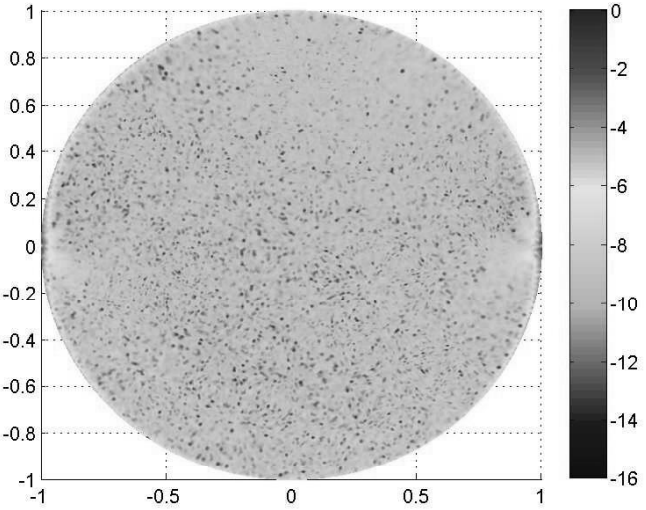

Figure 4: *Error distribution against the log-absolute error; Dirichlet boundary condition is imposed on* $\partial\Omega$.

10^{-10}) is used to generate boundary data. We consider two cases: first, $\Gamma_0 = \partial\Omega$, $\Gamma_1 = \emptyset$, and then $\Gamma_0 = \partial\Omega \cap \{y < 0\}$, $\Gamma_1 = \partial\Omega \cap \{y \geq 0\}$, respectively, for Dirichlet and mixed boundary conditions. In both cases, if not set-up properly, the MFS approximation will be severely polluted by Gibbs oscillations.

Since the exact solution is discontinuous on boundary, it is not possible to observe convergence in terms of ε_∞. Instead, the error ε_2 is evaluated with 40257 nodes. With Dirichlet boundary data only, the proposed search yields $\varepsilon_2 = 5.52E-3$; for instance, see Figure 4 for the corresponding error distribution. Away from the two jumps on boundary, the residual stays small rather uniformly inside the domain. For the mixed boundary condition case, we get $\varepsilon_2 = 3.62E-2$. From the error distribution in Figure 5, the reconstruction error gradually increases as we go towards the Neumann boundary.

5 Conclusion

We proposed a search algorithm to seek for a quasi-optimal setting for the method of fundamental solutions. The parameters to be searched are the number of source points and the source distances. A series of examples—including globally harmonic functions and discontinuous functions, and Dirichlet and mixed boundary conditions—are provided. These examples show the robustness of the proposed method. Also they provide a useful source of nontrivial test examples for researchers in the area.

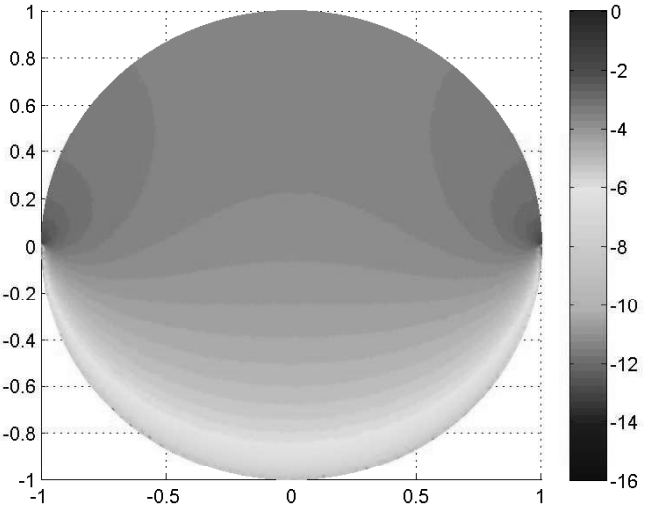

Figure 5: *Error distribution against the log-absolute error; Neumann boundary condition is imposed to the TOP semicircle* Γ_1*, Dirichlet to the rest.*

Acknowledgements

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