Engineering Analysis with Boundary Elements 35 (2011) 42–46

Contents lists available at ScienceDirect

Engineering Analysis with Boundary Elements

journal homepage: www.elsevier.com/locate/enganabound

Optimality of the method of fundamental solutions

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A R T I C L E I N F O

Article history:
Received 7 February 2010
Accepted 9 June 2010
Available online 2 July 2010

Keywords:
Effective-condition-number
Laplace equation
MFS

A B S T R A C T

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): 637-43], 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

$$\Delta u = 0 \quad \text{in } \Omega \subset \mathbb{R}^2,$$

$$\partial_n^{(k)} u = f_k \quad \text{on } \Gamma_k \subset \partial\Omega,\ k \in \{0,1\}, \tag{1}$$

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 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 $\Delta f_0 = 0$ 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 $\tilde{\Omega} \supset \Omega$ 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 $\partial\tilde{\Omega}$. The MFS

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doi:10.1016/j.enganabound.2010.06.002

approximates the solution of (1) by

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

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

$$\alpha_0 + \sum_{j=1}^{N} \alpha_j s_j(x_i) = f_0(x_i) \quad \text{for } x_i \in \Gamma_0,$$

$$\sum_{j=1}^{N} \alpha_j \partial_n s_j(x_i) = f_1(x_i) \quad \text{for } x_i \in \Gamma_1. \tag{3}$$

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

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

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 pre-defined 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

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

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

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 $\partial\tilde{\Omega}$ 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 $\partial\Omega$ ($\partial\tilde{\Omega}$). Unless otherwise mentioned, we start the first D-Search with $N=100$ and a fixed