Some Comments on the Ill-conditioning of the Method of Fundamental Solutions

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Abstract

In this paper we consider the accuracy and stability of implementing the Method of Fundamental Solutions. In contrast to the results shown in [5], we find that Gaussian elimination can be used reliably to solve the MFS equations and the use of the singular value decomposition shows no improvement over Gaussian elimination provided that the boundary condition is non-noisy. However, for noisy boundary conditions, there is evidence that the singular value decomposition with truncation is more accurate than Gaussian elimination.

Keywords: Method of fundamental solutions, ill-conditioning, singular value decomposition.

1 Introduction

In recent years there has been growing interest in using meshless methods for the numerical solution of partial differential equations (PDEs). A popular method of this type is the Method of Fundamental Solutions (MFS) [1, 2, 3] which may be viewed as a variant of the Boundary Element Method (BEM). In this method an approximate solution to an elliptic PDE

$$Lu = 0 \tag{1}$$

is represented in the form

$$u_N = \sum_{j=1}^{N} a_j G\left(P_j, Q\right) + h\left(P\right) \tag{2}$$

where $G\left(P, Q\right)$ is a fundamental solution of L; i.e., $G\left(P, Q\right)$ satisfies

$$LG\left(P, Q\right) = \delta\left(P - Q\right) \tag{3}$$

where $\delta\left(P - Q\right)$ is the Dirac delta function and h satisfies

$$Lh = 0. \tag{4}$$

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The points $\{P_j\}_{j=1}^N$ are generally chosen in the complement of the physical domain of the problem. Depending on L, it may be that $h = 0$. The constants $\{a_j\}_{j=1}^N$ and h are then chosen to satisfy the boundary conditions in some sense. If the boundary conditions are satisfied by collocation, this gives rise to a set of linear equations which can become highly ill-conditioned. Although this ill-conditioning of the system seems to have a minimal affect on the accuracy of the solution, it is of interest to see if standard methods for mitigating ill-conditioning, such as the singular value decomposition (SVD) or Tikhonov regularization can or should be used to mitigate the effect of the ill-conditioning. To the best of our knowledge, this problem was first studied by Kitagawa [4] who proposed using the SVD to understand the ill-conditioning of the MFS equations. This was recently reconsidered by Ramachandran [5] whose numerical experiments show that direct solution of the MFS equations by Gaussian elimination can be quite unreliable and that the truncated Singular Value Decomposition (TSVD) enables one to overcome this difficulty. In this paper, we reevaluate some of the results in [5] and find that his conclusions regarding the instability of Gaussian elimination is not entirely warranted. We further discover the argument in [5] is valid for noisy boundary conditions.

The structure of the paper is as follows. In Section 2 we outline the MFS for the two-dimensional Laplace equation and describe known theoretical results concerning the convergence and stability of the method. In particular, we argue that there is a trade-off between convergence and stability determined by the radius of the fictitious circle. This is demonstrated computationally, but we are able to show that the critical radius is significantly larger from that found in [5]. In Section 3 we examine the SVD as a possible remedy for the ill-conditioning and find, in Section 4, somewhat surprisingly, that the SVD solution differs little from the results obtained by Gaussian eliminations. Hence, it appears from these results, that Gaussian elimination can be reliably used to solve the MFS equations. This agrees with previous, but less formal approaches to the problem. In Section 5 we draw conclusions and discuss directions for future research.

2 The Method of Fundamental Solutions (MFS)

We consider the solution of the boundary value problem

$$\begin{cases} \dfrac{\partial^2 u(P)}{\partial x^2} + \dfrac{\partial^2 u(P)}{\partial y^2} \equiv \Delta u = 0, \ P \in \Omega, \\ Bu(P) = g(P), \ P \in \partial\Omega, \end{cases} \tag{5}$$

where Ω is a bounded simply connected domain in $\mathbb{R}^2$ and $\partial\Omega$ is the boundary of Ω. B is a boundary operator, generally of the form

$$Bu(P) = \alpha(P) u(P) + \beta(P) \frac{\partial u(P)}{\partial n} \tag{6}$$

where $\alpha(P), \beta(P)$ are piecewise continuous functions on $\partial\Omega$ and $\partial u/\partial n$ is the outward normal derivative of u at $P \in \partial\Omega$ when $\partial\Omega$ is sufficiently smooth and $g(P), P \in \partial\Omega$ is a given known piecewise continuous boundary function. If $\alpha(P) \neq 0$ and $\beta(P) = 0$, we have Dirichlet boundary condition, while if $\alpha(P) = 0$ and $\beta(P) \neq 0$, then we have Neumann boundary condition. Generally, B in (6) allows for both Robin and mixed boundary conditions. For now we focus on the particular case where $\partial\Omega$ is analytic and we have mixed boundary conditions. Then, (5)-(6) becomes

$$\Delta u\left(P\right)=0,\ P\in\Omega \tag{7}$$

$$u\left(P\right)=g_1\left(P\right),\ P\in\Gamma_1 \tag{8}$$

and

$$\frac{\partial u\left(P\right)}{\partial n}=g_2\left(P\right),\ P\in\Gamma_2 \tag{9}$$

where $\partial\Omega=\Gamma_1\cup\Gamma_2$ and $\Gamma_1\cap\Gamma_2=\varnothing$. In this case it is known that if $g_1\left(P\right)$ and $g_2\left(P\right)$ are continuous and satisfy suitable compatability conditions that (7)-(9) has a unique analytic solution for $P\in\Omega$. Numerous methods, such as the finite element, boundary element and a variety of domain-based mesh-reduced methods are available for this purpose. However, despite years of research, it is still difficult to obtain highly accurate numerical results with these methods. An alternative meshless method which has become increasingly popular in recent years is the Method of Fundamental Solutions first introduced by Kupradze and Aleksidze in 1964 [6]. As indicated in the Introduction, in this case the solution is represented as

$$u_N\left(P\right)=a_0+\sum_{j=1}^{N}a_j\log\left\|P-Q_j\right\| \tag{10}$$

where $\|\cdot\|$ is the Euclidean norm in $\mathbb{R}^2$ and $-\log\|P-Q\|/2\pi$ is the fundamental solution of $\Delta u=0$. For the examples in this paper, we have found it sufficient to take $a_0=0$.

The source points $\{Q_n\}_{j=1}^{N}$ are chosen in the exterior of Ω. The constants $\{a_j\}_{j=1}^{N}$ are chosen to satisfy the boundary condition in some sense. Typically, this is done by either least squares or collocation. Generally, collocation is easier to use and can produce highly accurate solutions, sometimes, almost achieving machine precision. This is the approach chosen in this paper.

Hence, let $\{Q_k\}_{k=1}^{N}$ be N points on $\partial\Omega$. Then $\{a_j\}_{j=1}^{N}$ are chosen to satisfy

$$u_N\left(P_k\right)=g_1\left(P_k\right),\ P_k\in\partial\Omega,1\leq k\leq m, \tag{11}$$

$$\frac{\partial u_N\left(P_k\right)}{\partial n}=g_2\left(P_k\right),\ P_k\in\partial\Omega,m+1\leq k\leq N. \tag{12}$$

Then $\{a_j\}_{j=1}^{N}$ satisfy the linear equations

$$\sum_{j=1}^{m}a_j\log\left\|P_j-Q_k\right\|=g_1\left(P_k\right),\ 1\leq k\leq m, \tag{13}$$

$$\sum_{j=m+1}^{N}a_j\frac{\partial}{\partial n}\log\left\|P_j-Q_k\right\|=g_2\left(P_k\right),\ m+1\leq k\leq N. \tag{14}$$

The points $\{P_k\}_{k=1}^{m}$ are chosen to satisfy (8) while the $\{P_k\}_{k=m+1}^{N}$ are chosen to satisfy (9). The above equations form a system of $N\times N$ equations.

Using this approach, a number of practical issues arise; where should one choose the source and collocation points and how large should N be chosen? As a guide to answering these questions, we have relied on the theoretical results in [7, 8] and those of Katsurada in [9]. In

[8] Cheng studied the Dirichlet case where the domain Ω is a circle of radius r and the sources are placed uniformly around a circle of radius $R > r$. The collocation points are also chosen uniformly spared around the boundary $\partial\Omega$. In this case it was shown that the error

$$\max_D |u - u_N| \le c\,(r/R)^N \tag{15}$$

where c is a constant independent of N. Hence, the error decreases exponentially as $N \to \infty$ and $R \to \infty$. For purposes of efficiency, it is generally better to use a moderate value of N and try to take R as large as possible. Unfortunately, this presents problems as the condition number of $\mathbf{A}$ (see Section 3) increases like e^R. Hence, one expects that for some value of R that the round-off error will dominate the truncation error and the overall error tends to decrease and then increase for large R.

Because of this ill-conditioning, there have been doubts about the ability of standard linear equation solvers such as Gaussian elimination to accurately solve the MFS equations. As a result, it has been suggested that more sophisticated methods, such as the singular value decomposition (SVD) or Tikhonov regularization [10] be used to produce more reliable solutions to (13)-(14). In particular, Ramachandran [5] shows that Gaussian elimination works only for fairly small values of R and hence SVD is needed to solve (13)-(14) reliably. As we show below, these results appear to be pessimistic and Gaussian elimination can be used to solve (13)-(14) at least as accurately as the SVD. Consequently, Gaussian elimination can be used to obtain accurate solutions to the MFS equations.

3 SVD and Truncated SVD

Before presenting our numerical results, we give a brief discussion of the singular value decomposition. As is well known, an $N \times N$ matrix $\mathbf{A}$ can be decomposed as

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^T \tag{16}$$

where $\mathbf{U}$ and $\mathbf{V}$ are orthogonal matrices and $\mathbf{D}$ is a diagonal matrix with diagonal elements

$$\sigma_1 \ge \sigma_2 \ge \cdots \ge \sigma_N \ge 0 \tag{17}$$

where $\sigma_i, 1 \le i \le N$ are called the *singular values* of $\mathbf{A}$ and

$$\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_N]\,, \tag{18}$$

and

$$\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_N]\,, \tag{19}$$

are matrices of right and left singular vectors of $\mathbf{A}$. The decomposition (16) is called the *singular value decomposition* (SVD) of $\mathbf{A}$.

Using (16) the equations $\mathbf{A}\mathbf{x} = \mathbf{y}$ can be solved in the following form

$$\mathbf{x} = \sum_{i=1}^{N} \frac{\mathbf{u}_i^T \mathbf{y}}{\sigma_i} \mathbf{v}_i. \tag{20}$$

Typically, the ill-conditioning of $\mathbf{A}$ manifests itself with the presence of small singular values of $\mathbf{A}$. In fact, the condition number of $\mathbf{A}$ is defined by

$$\kappa(\mathbf{A}) = \sigma_N/\sigma_1. \tag{21}$$

Hence, to mitigate the ill-conditioning one often truncates (20) by dropping all terms with $\sigma_i < \epsilon$ for some preassigned values of ϵ. In this case, $\mathbf{x}$ is approximated by

$$\tilde{\mathbf{x}} = \sum_{i=1}^{M} \frac{\mathbf{u}_i^T \mathbf{y}}{\sigma_i} \mathbf{v}_i, \tag{22}$$

where $\sigma_i \geq \epsilon, i = 1, 2, ..., M\,(< N)$.

The expansion in (16) is called the *truncated singular value decomposition* (TSVD) of $\mathbf{A}$. The value of ε can be chosen arbitrarily or by some more formal method such as the L-curve or cross-validation [11, 12]. In [5], ϵ appears to have been chosen as $\epsilon = 10^{-4}$ which we believe is too large to provide an accurate representation of the solution. Despite the expectation that the SVD should improve the MFS algorithm, numerical results given below show no substantial improvement over Gaussian elimination. Again this contrasts with the results given in [5].

4 Numerical Results

In this Section, we present three numerical examples. Throughout this section, the numerical results were obtained using Fortran with IMSL subroutines which include the SVD solver DLSVRR. Due to the maximum principle, the absolute maximum error occurs on the boundary. Hence, we choose 121 test points that are uniformly distributed on $\partial\Omega$ for the evaluation of the absolute maximum error. For convenience, we choose the same number of collocation points and source points which are uniformly distributed (in term of angle) on the physical boundary and the fictitious boundary respectively. Furthermore, we choose the circle with center at $(0, 0)$ with radius r as the fictitious boundary.

Example 1 In this example, we revisit the problem considered in [5]. Here, we consider the Laplace equation with Dirichlet boundary conditions; i.e.,

$$u(x, y) = e^x \cos y, \quad (x, y) \in \partial\Omega,$$

where

$$\partial\Omega = \left\{ (r\cos\theta, r\sin\theta) : r = \sqrt{\cos 2\theta + \sqrt{2 - \sin^2 2\theta}}, 0 \leq \theta \leq 2\pi \right\}.$$

Since the imposed boundary condition is harmonic, the exact solution is given by $u(x, y) = e^x \cos y$.

First, we choose 40 collocation and source points on $\partial\Omega$ and the fictitious boundary respectively. In Table 1, we show the absolute maximum errors using SVD and direct Gaussian elimination. In the SVD, we choose all of the singular values ($M = 40$). We found that the numerical results using these two approaches were almost identical. There is no evidence that the SVD is superior to Gaussian elimination. This is a direct contradiction to the results obtained in [5] where the author claimed that the solution diverged for large r using Gaussian

Table 1: Comparison of Gaussian elimination and SVD

Source radius r	L_∞ (Gaussian)	L_∞ (SVD)
2.00	$2.00E-4$	$2.00E-4$
3.00	$1.20E-9$	$1.17E-9$
5.00	$4.85E-10$	$7.54E-10$
8.00	$5.68E-9$	$2.26E-9$
10.00	$9.92E-10$	$4.45E-10$
20.00	$3.18E-7$	$1.02E-7$

elimination. Note that we produced the similar results in Table 1 using the MATLAB which is being used in [5].

Next, we consider mixed boundary conditions. Let $\partial\Omega = \Gamma_1 \cup \Gamma_2$. As shown in Figure 1, we impose the Neumann condition on Γ_1, which contains the first quadrant, and Dirichlet conditions on Γ_2. The boundary conditions are imposed in such a way so that the exact solution is $u(x, y) = e^x \cos y$.

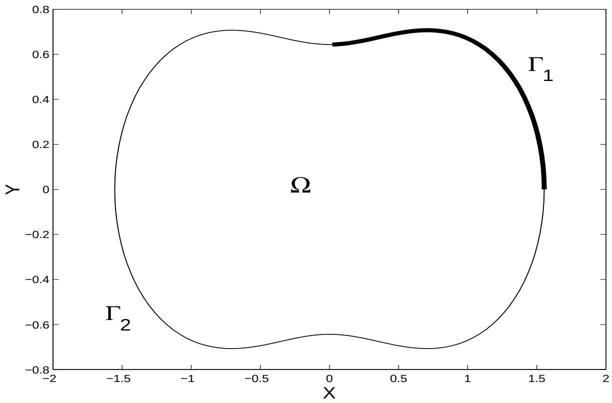

Figure 1: Profile of the Neumann and Dirichlet boundary conditions.

We choose 200 collocation and source points and perform the same test as shown above. We denote e, e_x and e_y the absolute maximum errors of u, u_x and u_y respectively; i.e.,

$$e = \|u - u_N\|_\infty, \quad e_x = \|u_x - u_{N,x}\|_\infty, \quad e_y = \|u_y - u_{N,y}\|_\infty$$

where $u_{N,x} = \partial u_N/\partial x$ and $u_{N,y} = \partial u_N/\partial y$.

Again, as shown in Table 2, it does not seem to be that the SVD is superior to Gaussian elimination.

Example 2 To study the effect of the TSVD on the solution accuracy, we again consider the Laplace equation with mixed boundary conditions. Let

$$\partial\Omega = \{(r\cos\theta, r\sin\theta) : r = e^{\sin\theta}(\sin^2(2\theta)) + e^{\cos\theta}(\cos^2(2\theta))\}.$$

Table 2: Absolute maximum errors for e, e_x, and e_y for mixed boundary conditions

	SVD			Gaussian		
r	e	e_x	e_y	e	e_x	e_y
4	$6.48E-14$	$1.29E-13$	$1.65E-13$	$8.09E-14$	$6.53E-14$	$6.58E-13$
6	$6.87E-13$	$2.95E-12$	$2.92E-12$	$7.87E-13$	$6.47E-12$	$5.75E-12$
8	$1.99E-11$	$5.24E-11$	$5.05E-11$	$2.15E-11$	$1.64E-10$	$1.64E-10$

The boundary $\partial\Omega$ is an amoeba-like irregular shape. (See Figure 2). The boundary conditions are given by

$$u(x,y) = e^x \cos y, \quad (x,y) \in \Gamma_1,$$
$$\frac{\partial}{\partial \mathbf{n}} u(x,y) = (e^x \cos y)\,\mathbf{n}_x - (e^x \sin y)\,\mathbf{n}_y, \quad (x,y) \in \Gamma_2,$$

where $\Gamma_2 = \partial\Omega$ with $0 \le \theta < \pi$, and $\Gamma_1 = \partial\Omega$ with $\pi \le \theta < 2\pi$. As shown in Figure 2, the Neumann condition is imposed on the upper half of the amoeba-like curve, and the Dirichlet boundary condition on the lower half.

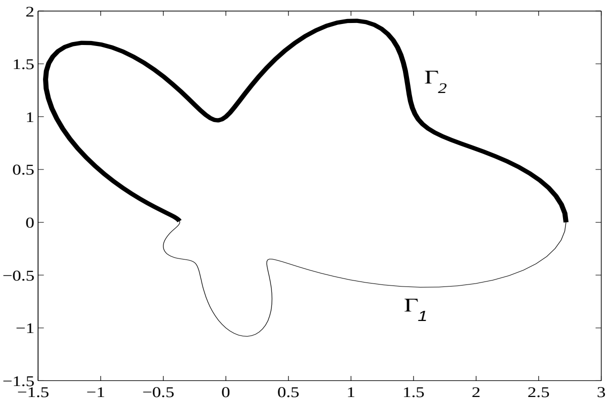

Figure 2: Neumann and Dirichlet boundary conditions.

We first choose 100 collocation and source points on $\partial\Omega$ and the fictitious circle with $r = 8$ respectively. In Figure 3, we show the absolute maximum errors of e, e_x, and e_y versus the effective rank of $\mathbf{A}$, the number of singular values being used. In Figure 3, we also present the distribution of the singular values. There seems no significant difference in accuracy using more than 40 singular values. This indicates that the SVD truncation error and round-off error have little effect on the accuracy.

We repeated the above test using 200 collocation and source points as above. In this case, we choose the radius of the fictitious circle $r = 4$. The results are shown in Figure 4. We observe that we can achieve near machine precision. Both cases reveal similar behavior in the distribution of errors and singular values.

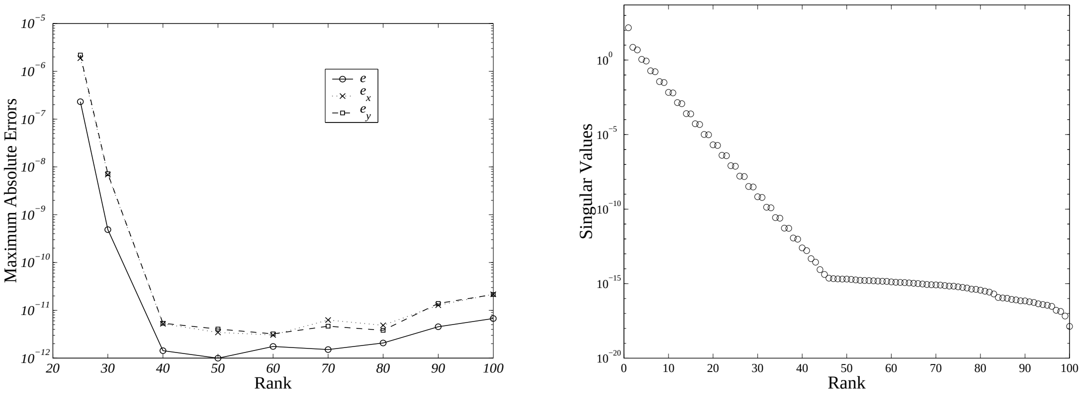

Figure 3: Profiles of e, e_x, e_y (left) and distribution of singular values (right) using 100 collocation and source points.

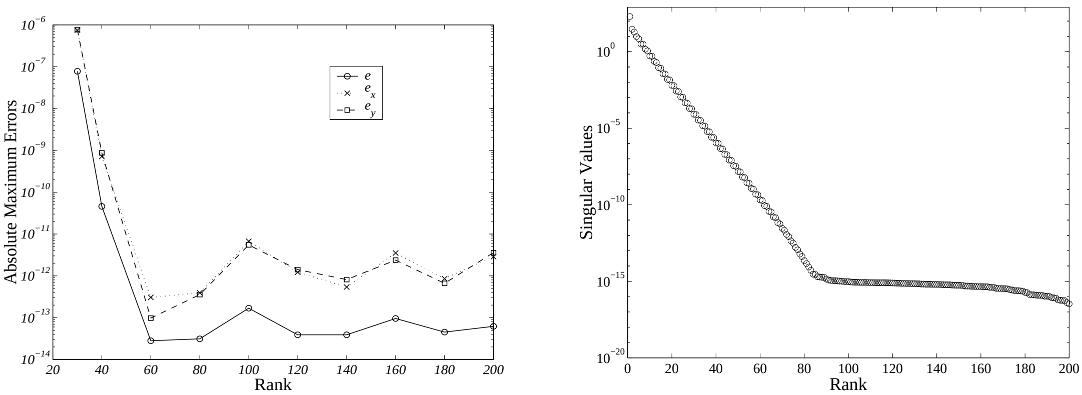

Figure 4: Profiles of e, e_x, e_y (left) and distribution of singular values (right) using 200 collocation and source points.

In Table 3, we show again that there is no significant difference between Gaussian elimination and the SVD using 200 collocation and source points. In [13], the authors also claimed that the source points should be located close to the boundary for the Neumann condition and away from the boundary for the Dirichlet condition. We have conducted numerous tests using various boundary shapes and conditions, and found no difficulty in using the circle as the fictitious boundary.

Example 3 We consider the same problem as Example 2 by adding some random noise to the boundary conditions.

$$u(x,y) = e^x \cos y + \delta, \quad (x,y) \in \Gamma_1,$$
$$\frac{\partial}{\partial \mathbf{n}} u(x,y) = (e^x \cos y)\,\mathbf{n}_x - (e^x \sin y)\,\mathbf{n}_y + \delta, \quad (x,y), \in \Gamma_2,$$

Table 3: Comparison of Gaussian elimination, SVD and TSVD

Source radius r	L_∞ (Gaussian)	L_∞ (SVD)	L_∞ (TSVD) w/ 85
4	$4.70E-11$	$6.22E-14$	$2.48E-13$
5	$1.88E-13$	$4.03E-13$	$1.13E-13$
6	$1.67E-13$	$6.68E-13$	$1.57E-13$
7	$3.99E-12$	$2.25E-12$	$8.64E-13$

where $\delta = \varepsilon \times Rand$. We use the uniform random number generator to produce random numbers $Rand$ in $[-1, 1]$. Here ε denotes the level of the noise. Similarly to the last example, we choose 200 collocation and source points. We choose 60 singular values for the TSVD. The noise level ε is set to be at the 1% level. The absolute maximum errors for e and e_x versus source radius are shown in Figure 5. We ignore the plot of e_y since it behaves similar to the plot of e_x. It is clear that the TSVD is superior to the SVD and Gaussian elimination. Again, there is little difference among Gaussian elimination, the SVD and TSVD.

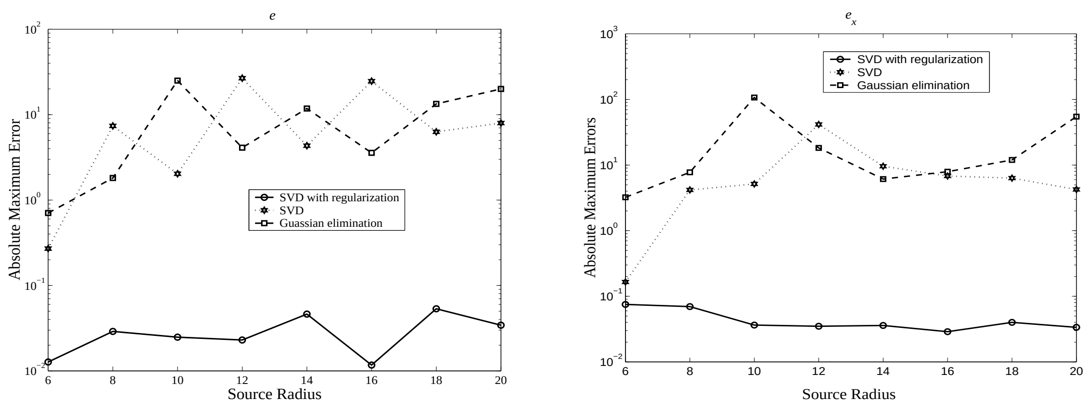

Figure 5: Absolute maximum errors of e (left) and e_x (right).

In [14, 15], the authors have discussed the details on how to choose the regularization parameters using various techniques. However, we found the simple TSVD is sufficient to produce good results in our cases. We suggest choosing a sufficiently large amount of collocation and source points in the formulation and then we can comfortably cut-off half of the singular values without loss of accuracy. Using SVD, we know how to eliminate the smaller singular values. In Gaussian elimination, it is not clear how to remove the redundant source points. Using TSVD, the radius of the fictitious circus is no longer an issue. This is due to the fact that the larger the radius of the source circle, the worse the ill-conditioning. However, since the ill-conditioning is due to the small singular values which are in descending order, it is rather easy to remove them. The price we have to pay for the convenience of choosing the source radius is to choose much more source points than we need. In the last and current example, we found that only 60 out of the 200 singular values were enough to produce accurate results.

5 Conclusions

We have reexamined some results in [5] regarding the use of Gaussian elimination and the SVD for solving the ill-conditioned MFS equations. In contrast to the results in [5], we show that the SVD is not more reliable than Gaussian elimination for solving these equations for non-noisy boundary conditions. Since Gaussian elimination is cheaper than SVD, we recommend that it can be used to efficiently and accurately to implement the MFS. For noisy boundary conditions, TSVD is clearly superior to Gaussian elimination. In this paper we also suggest how to choose the number of source points and the radius of the source circle using TSVD. Since our results are given only for the two-dimensional Laplace-equation, future work will focus on three-dimensional problems and other equations such as the Poisson equation, biharmonic and Helmholtz equations.

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References

[1] Cho HA, Golberg MA, Muleshkov AS, Li X. Trefftz Methods for Time Dependent Partial Differential Equations. CMC 2004;1:1-37.

[2] Fairweather G, Karageorghis A. The method of fundamental solution for elliptic boundary value problems, Advances in Computaitonal Mathematics 1998;9:69-95.

[3] Golberg MA, Chen CS (1998). The method of fundamental solutions for potential, Helmholtz and diffusion problems. In: Golberg MA, editor. Boundary Integral Methods - Numerical and Mathematical Aspects. Computational Mechanics Publications; 1998. p. 103-176.

[4] Kitagawa T. On the numerical stability of the method of fundamental solution applied to Dirichlet problem. Japan Journal of Applied Mathematics 1988;5:123-133.

[5] Ramachandran PA. Method of fundamental solutions: singular value decomposition analysis. Communications in Numerical Methods in Engineering 2002;18:789-801.

[6] Kupradze VD, Aleksidze MA. The method of functional equations for the approximate solution of certain boundary value problems. U.S.S.R. Computational Mathematics and Mathematical Physics 1964;4:82-126.

[7] Bogomolny A. Fundamental solutions method for elliptic boundary value problems. SIAM Journal on Numerical Analysis 1985;22:644-669.

[8] Cheng RSC Delta-Trigonometric and Spline Methods using the Single-Layer Potential Representation. Ph.D. dissertation, University of Maryland; 1987.

[9] Katsurada M. Asymptotic error analysis of the charge simulation method in Jordan regions with an analytic boundary. Journal of Faculty of Science of the University, Tokyo, Section 1A. Mathematics 1990;37:635-657.

[10] Tikhonov AN, Arsenin VY. On the solution of ill-posed problems. New York: John Wiley and Sons; 1977

[11] Hansen PC. Analysis of discrete ill-posed problems by means of the L-curve. SIAM Review 1992;34:561-580.

[12] Hansen PC, O'Leary DP. The use of the L-curve in the regularization of discrete ill-posed problems. SIAM Journal of Scientific Computing 1993;14:1487-1503.

[13] Balakrishnan K, Ramachandran PA. A particular solution Trefftz method for non-linear Poisson problems in heat and mass transfer. Journal of Computational Physics 1999;150:239-267.

[14] Hon YC, Wei T. The method of fundamental solutions for solving multidimensional inverse heat conduction problems. CMES 2004;7:119-132.

[15] Jin B. A meshless method for the Laplace and biharmonic equations subjected to noisy boundary data. CMES 2005;6:253-262.