A new investigation into regularization techniques for the method of fundamental solutions

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Abstract

This study examines different regularization approaches to investigate the solution stability of the method of fundamental solutions (MFS). We compare three regularization methods in conjunction with two different regularization parameters to find the optimal stable MFS scheme. Meanwhile, we have investigated the relationship among the condition number, the effective condition number, and the MFS solution accuracy. Numerical results show that the damped singular value decomposition under the parameter choice of the generalized cross-validation performs the best in terms of the MFS stability analysis. We also find that the condition number is a superior criterion to the effective condition number.

Keywords: Method of fundamental solutions; Regularization technique; Regularization parameter; Effective condition number

1. Introduction

In recent years, the method of fundamental solutions has rightfully received a great deal of attention by applied mathematicians and engineers in dealing with a variety of engineering problems\cite{2,4,6–8,14}. This method is a boundary-type meshless method with its merits being integration-free, spectral convergence, and easy to use. Despite these merits, we find that the convergence curves of the MFS numerical solution oscillate when a large number of boundary points are used. This may partially due to the ill-conditioned coefficient matrix\cite{16,17}. Therefore, it is of interest to see if regularization methods, such as the damped singular value decomposition (DSVD), the truncated singular value decomposition (TSVD) or the Tikhonov regularization (TR), can or should be used to mitigate the ill-conditioned effect.

To the best of our knowledge, Kitagawa\cite{15} first used the singular value decomposition (SVD) to deal with the solution of the ill-conditioned MFS equations. Based on the SVD, Ramachandran\cite{21} used an alternative solution procedure to illustrate that the numerical results are extremely accurate and relatively independent of the location of the source points. However, Chen et al.\cite{3} showed that the SVD is not more reliable than Gaussian elimination in...
solving the discretization algebraic equations with non-noisy boundary conditions. But for noisy boundary conditions, the TSVD is clearly superior to Gaussian elimination. Wei et al. [29] made a comprehensive comparison of various regularization techniques in the MFS solution of inverse Cauchy problems. Recently, Drombosky et al. [5] used the so-called effective condition number which considers the right-hand side vector to investigate the ill-conditioned MFS coefficient matrix. It is concluded that the condition number is an inferior criterion to the effective condition number in the estimate of the solution accuracy.

All the above-mentioned studies, however, are not involved with the detailed investigation into the convergence behaviors of the MFS solution for direct problems. In this study, we examine various regularization methods in the MFS solution of various benchmark direct problems [9,10,26,28]. As a further investigation based on the work reported in Ref. [5], we also analyze the relationship among the condition number, the effective condition number, and the MFS solution accuracy. Our numerical results show that the MFS combined with the DSVD under parameter choice of the generalized cross-validation (GCV) is an optimal stable method in dealing with direct problems. For the cases that the condition number is smaller than $10^{16}$, we find that the condition number is a superior index of accuracy estimate to the effective condition number.

The structure of the paper is as follows. In Section 2, we review the key idea of the MFS. Three regularization techniques and two approaches for the parameter choice are described in Section 3. Followed by Section 4, three benchmark numerical examples are tested to examine the performances of all above-mentioned regularization methods. Section 5 concludes this study with some remarks.

2. Method of fundamental solutions

We consider the boundary value problem:

\[ Lu(x, y) = 0 \quad \text{in} \quad \Omega, \]
\[ u(x, y) = f(x, y) \quad \text{on} \quad \Gamma_D, \]
\[ \frac{\partial u(x, y)}{\partial n} = g(x, y) \quad \text{on} \quad \Gamma_N \]

where \( L \) is a linear elliptic partial differential operator, \( \Omega \) represents a bounded simply connected domain in \( \Re^2 \) and \( \partial \Omega = \Gamma_D \cup \Gamma_N \) its boundary, \( \partial u/\partial n \) denotes the outward normal derivative.

In this paper, we consider three linear elliptic partial differential operators, the fundamental solutions of Eq. (1) for different operators are given by:

\[ u_L = -\frac{1}{2\pi} \ln(r(X, Y)), \quad X \in \partial \Omega, \quad Y \in \Re^2 \setminus \partial \Omega, \]

for Laplace equation,

\[ u_h = \frac{1}{2\pi} Y_0(\lambda r(X, Y)), \quad X \in \partial \Omega, \quad Y \in \Re^2 \setminus \partial \Omega, \]

for Helmholtz equation and

\[ u_{mh} = \frac{1}{2\pi} K_0(\lambda r(X, Y)), \quad X \in \partial \Omega, \quad Y \in \Re^2 \setminus \partial \Omega, \]

for modified Helmholtz equation, where \( r(X, Y) = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} \) represents the distance between the collocation point \( X = (x_1, y_1) \) and the source point \( Y = (x_2, y_2) \), \( Y_0 \) and \( K_0 \) stands for the Bessel function and the modified Bessel function of the second kind of order zero, respectively.

Using the fundamental solution, we can approximate the solution of respective Eq. (1) by

\[ u(X_i) = \sum_{j=1}^{N} a_j u(r(X_i, Y_j)), \]
where \( a_i \) are the unknown coefficients. By collocating boundary conditions Eqs. (2) and (3), we have
\[
f(X_i) = \sum_{j=1}^{N} a_j u(r(X_i, Y_j)) \quad X_i \in \Gamma_D.
\]
\[
g(X_i) = \sum_{j=1}^{N} a_j \frac{\partial u(r(X_i, Y_j))}{\partial n} \quad X_i \in \Gamma_N.
\]

The resulting matrix expression of the MFS discretization equation to determine the coefficients \( \alpha = (a_1, a_2, \ldots, a_N) \) is made up of Eqs. (7)–(9), namely,
\[
A\alpha = b
\]
where \( A = (A_{ij}) \) is the MFS coefficient matrix.

The coefficient matrix \( A \) in above Eq. (10) is often severely ill-conditioned. In recent decades, some regularization methods have been proposed to remedy the instability and accuracy loss in the solution of such ill-conditioned matrix equations [25,26,13,11,27,19,20,31]. In this paper, we consider three commonly used regularization methods based on the SVD to study the stability and accuracy of the MFS.

3. Regularization methods

Before presenting the regularization methods, we give a brief discussion of the SVD. The SVD of the \( N \times N \) matrix \( A \) is a decomposition of the form
\[
A = W\Sigma V^T,
\]
where \( W = [w_1, w_2, \ldots, w_N] \) and \( V = [v_1, v_2, \ldots, v_N] \) are matrices with orthogonal columns, \( W^TW = V^TV = I_N \), and \( \Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_N) \) has non-negative diagonal elements appearing in non-increasing order such that
\[
\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_N \geq 0,
\]
where \( \sigma_i \) represents the singular values of \( A \) while the vectors \( W \) and \( V \) are the left and right vectors of \( A \). Then the right side of Eq. (10) \( b \) can be written as
\[
b = \sum_{i=1}^{N} \beta_i w_i,
\]
and the solution of Eq. (10) has the formula:
\[
\alpha = \sum_{i=1}^{N} \frac{w_i^T b v_i}{\sigma_i}.
\]

The conventional \( L^2 \) condition number is defined as \( \text{Cond}(A) = \sigma_1/\sigma_N \), where \( \sigma_1 \) and \( \sigma_N \) are the largest and smallest singular value of \( A \). In order to take the right hand vector into account, we introduce the effective condition number for the matrix equation \( A\alpha = b \) defined as [5,30]
\[
\text{ECN}(A, b) = \frac{||b||_2}{\sigma_N \sqrt{(\beta_1/\sigma_1)^2 + (\beta_2/\sigma_2)^2 + \cdots + (\beta_N/\sigma_N)^2}}.
\]

The other kinds of effective condition numbers are refereed to Refs. [1,18].

3.1. Regularization methods

Using the SVD, this study considers three regularization methods, that is, the TR, TSVD and DSVD [31,32].
**TR** [26]: The TR technique consists of seeking a solution which minimizes a criterion made up of the sum of two components. The first one is a possibly weighted least square term while the second one is a quadratic penalty term on the solution, that is

\[
\min \{||A\alpha - b||_2^2 + \xi^2||I\alpha||_2^2\},
\]

(16)

where \( || . ||_2 \) denotes the Euclidean norm, \( I \) symbolizes the identity matrix and \( \xi \) is the regularization parameter which often controls the relative weight of the penalty term in the criterion. When the parameter \( \xi = 0 \), Eq. (16) degenerates to the least squares problem.

Based on the SVD, the Tikhonov regularized solution can be expressed as

\[
\alpha = \sum_{i=1}^{N} g_i \frac{w_i^T b v_i}{\sigma_i},
\]

(17)

where the Wiener weights are

\[
g_i = \frac{\sigma_i^2}{\sigma_i^2 + \xi^2}.
\]

(18)

**DSVD**: Instead of using the filter factors (18) in the TR, the DSVD introduces a smoother cut-off by means of filter factors \( g_i \) defined as

\[
g_i = \frac{\sigma_i}{\sigma_i + \xi}.
\]

(19)

These filter factors decay slower than the Tikhonov one and thus makes less filtering.

**TSVD** [22,11]: The basic idea of the TSVD is to impose additional requirement on the solution that its norm be small. This is achieved by neglection of the smallest singular value for its large contribution to the solution. Thus, the rank-\( K \) matrix \( A_K \) which is given as

\[
A_K = W\Sigma_K V^T = \sum_{i=1}^{K} w_i \sigma_i v_i^T, \quad K \leq N,
\]

(20)

where \( \Sigma_K = \text{diag}(\sigma_1, \ldots, \sigma_K, 0, \ldots, 0) \) equals to \( \Sigma \) with the smallest singular values to be replaced by zeros. By this, the condition number \( \text{Cond}(A_K) = \sigma_1/\sigma_K \) of the TSVD \( A_K \) will be small. Then the solution of Eq. (10) is defined by the following minimization problem:

\[
\min ||\alpha||_2 \text{ subject to } \min ||A_K \alpha - b||_2
\]

(21)

given by:

\[
\alpha^K = A_K^+ b = V\Sigma_K^+ W^T b = \sum_{i=1}^{K} \frac{w_i^T b v_i}{\sigma_i},
\]

(22)

where \( K \leq N \) is also a regularization parameter, \( A_K^+ \) is a pseudoinverse of \( A \) and \( \Sigma_K^+ = \text{diag}(\sigma_1^{-1}, \ldots, \sigma_K^{-1}, 0, \ldots, 0) \).

### 3.2. Regularization parameters

A proper choice of the regularization parameter is essential for the effectiveness of regularization methods applied to the ill-conditioned interpolation matrix equation. However, the optimal determination of a regularization parameter in general remains an open issue under intensive research. Here we briefly recall the two of the most widely used techniques, i.e., the LC and the GCV.

**LC for choosing the regularization parameter** [23]: Intuitively, the best regularization parameter should lie on the corner of the LC, defined as:

\[
L = \{\log ||\alpha\alpha||_2, \log ||Aa\alpha - b||_2 : \alpha \geq 0\}.
\]

(23)
This curve is usually referred to as the L-curve, because for a large class of problems it is shaped like the letter L. We note here that the LC is a continuous curve when the regularization parameter is real in the Tikhonov regularization and the DSVD. For regularization method with a discrete regularization parameter, such as in the truncated singular value decomposition, a finite set of points

$$\{\log ||a_\alpha||_2, \log ||Aa_\alpha - b||_2 : \alpha = 1, 2, \ldots, n\},$$

will be obtained and interpolated by a spline curve.

**GCV for choosing the regularization parameter:** The GCV estimates the optimal value of the regularization parameter by minimizing the functional

$$V(\alpha) = \frac{(1/N)||I - A(\alpha)||b||^2}{((1/N) \text{trace} (I - A(\alpha)))^2}.$$  

The influence matrix $A_\alpha$ is defined by the identity

$$Aa_\alpha = A(\alpha)b.$$  

The GCV has some computationally relevant properties. Moreover, it is a predictive mean-square error criteria, in the sense that it estimates the minimizer of the residual function

$$T(K) = \frac{1}{N}||A(\alpha_K - \alpha)||^2.$$  

Based on the above-mentioned approaches, we compare the performances of the MFS combined with six regularized methods and without regularization in the solution of the three benchmark examples in the following section.

### 4. Numerical results and discussions

To illustrate the solution stability for these regularization methods, this study tests the three different types of numerical examples. The average relative error ($L_2$ relative error) in the following figures is defined as [31]:

$$\text{RMSE} = \sqrt{\frac{1}{N_t} \sum_{j=1}^{N_t} \frac{|u(x_j, y_j) - \tilde{u}(x_j, y_j)|^2}{u(x_j, y_j)},}$$

for $|u(x_j, y_j)| \geq 10^{-3}$ and

$$\text{RMSE} = \sqrt{\frac{1}{N_t} \sum_{j=1}^{N_t} |u(x_j, y_j) - \tilde{u}(x_j, y_j)|^2},$$

for $|u(x_j, y_j)| < 10^{-3}$, where $i$ is the index of the tested point, $N_t$ represents the total number of tested points, $u(x_j, y_j)$ and $\tilde{u}(x_j, y_j)$ denote the exact solution and the numerical approximation, respectively. It is noted that the shape of the auxiliary curve has no obvious impact on the numerical results [8,24]. Thus, the source points are uniformly distributed on a circle surrounding the solution domain in the following examples. It is also noted that MATLAB regularization code developed by Hansen has been used in our computations [10].

#### 4.1. Case 1: Laplace equation

In this case, we consider the Laplace problem on $\Omega = \{(x, y)|0 < x < 1, 0 < y < 1\}$ under mixed boundary conditions with two Dirichlet edges ($x = 1, y = 1$) and two Neumann edges ($x = 0, y = 0$). The source points are uniformly distributed on a concentric circle surrounding the solution domain. Here, the radius $R = 3$ is considered. The analytical solution is taken to be $u(x, y) = \sin(x)\sinh(y) + \cos(x)\cosh(y)$.

The relative average error curves against boundary point numbers are displayed in Fig. 1. It can be seen that the convergence curve of the MFS with no regularization techniques oscillates when the boundary point number $N$ increases. By using the DSVD under the GCV parameter choice (GCV–DSVD), the MFS solution accuracy degrades by one order of magnitude, but the convergence curve is far more stable than the other methods. Although the LC–TSVD
is excellent for solving inverse problems with noisy boundary conditions [12], it fails to yield acceptable numerical approximation in this case.

Corresponding to the given results of GCV–DSVD in Fig. 1, the condition number and the effective condition number are given in Table 1. We can see that the relative average error relates very closely with the condition number rather than the effective condition number. More precisely, the solution accuracy of MFS combined with GCV–DSVD is inversely proportional to the condition number. Thus, the condition number can be viewed as an estimator of the MFS solution accuracy.

4.2. Case 2: Helmholtz equation

We consider the Helmholtz equation on a unit circular domain centered with the origin under wave number \( \lambda = \sqrt{2} \), and only Dirichlet boundary is considered. The source points are distributed evenly on a concentric circle with radius \( R = 3 \). The analytical solution is

\[
    u(x, y) = \sin(x) \cos(y).
\]

(28)

The relative average error curves against boundary point numbers are given in Fig. 2. The oscillation of the MFS convergence curve is not very high. Despite the solution accuracy of the GCV–DSVD is lower than the MFS, the convergence curve of the GCV–DSVD is far more stable. In stark contrast, all the three regularization method under the LC parameter choice perform very badly and fail to produce acceptable solutions.

Further referring to the GCV–DSVD results shown in Fig. 2, the condition number and the effective condition number are given in Table 2. We observe that the condition number is inversely proportional to the relative average error, but the relationship between the effective condition number and the relative average error is inconclusive.

4.3. Case 3: modified Helmholtz equation

The last case is to examine the modified Helmholtz equation under a complex-shaped physical domain, as shown in Fig. 3, only Dirichlet boundary condition is taken. The source points are distributed on a circle surrounding the solution

<table>
<thead>
<tr>
<th>( N )</th>
<th>Cond</th>
<th>ECN</th>
<th>RMSE</th>
</tr>
</thead>
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<tr>
<td>8</td>
<td>1.06 \times 10^3</td>
<td>5.23 \times 10^1</td>
<td>9.70 \times 10^{-3}</td>
</tr>
<tr>
<td>12</td>
<td>1.58 \times 10^5</td>
<td>4.79 \times 10^3</td>
<td>4.15 \times 10^{-5}</td>
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<tr>
<td>20</td>
<td>3.51 \times 10^8</td>
<td>1.20 \times 10^7</td>
<td>1.67 \times 10^{-8}</td>
</tr>
<tr>
<td>24</td>
<td>2.55 \times 10^9</td>
<td>8.69 \times 10^7</td>
<td>2.74 \times 10^{-9}</td>
</tr>
<tr>
<td>32</td>
<td>3.08 \times 10^{12}</td>
<td>1.05 \times 10^{11}</td>
<td>2.52 \times 10^{-12}</td>
</tr>
<tr>
<td>40</td>
<td>3.48 \times 10^{15}</td>
<td>1.19 \times 10^{14}</td>
<td>3.93 \times 10^{-14}</td>
</tr>
</tbody>
</table>
domain, and the radius $R = 2$ is considered. Corresponding to the wave number $\lambda = \sqrt{2}$, the analytical solution is given by

$$u(x, y) = e^{(x+y)}. \tag{29}$$

Fig. 4 shows the relative average error curve against boundary point numbers. It is found that the MFS with no regularization technique encounters oscillatory problem. The DSVD under parameter choice of the GCV or the LC exhibits smooth convergence curve and their accuracy are equal to the MFS with no regularization technique.

Almost all convergence curves in Fig. 4 have a corner corresponding to the same boundary point number $N = 57$. In Table 3, it is clear that the MFS solutions almost always achieve the best results ($\text{RMSE} \approx 10^{-15}$) which means the distance of the auxiliary curve has no obvious impact on the numerical results. In most situations allow the MFS to
achieve high accuracy, the highest effective condition number (ECN \approx 10^{16}) and the condition number (Cond \approx 10^{18}) are also produced.

Based on the foregoing results, one may guess that when the condition number is not very large (Cond < 10^{16}), the relationship between the condition number and the relative average error is inversely proportional.

### 5. Concluding remarks

This paper examines six different regularization methods in the MFS solution of various benchmark problems. Based on the foregoing numerical results and discussions in Section 4, we find that the MFS combined with the DSVD under the GCV parameter choice performs more stable than all the other methods. Meanwhile, we notice that the distance of the auxiliary curve has no obvious impact on the numerical results.

Despite of the excellent performance in solving inverse problems [12], the TSVD under the LC parameter choice fails to yield acceptable numerical approximation for problems tested in this study. We also observe that the condition number of the MFS coefficient matrix is inversely proportional to the solution accuracy. It is noted that the condition number is a superior criterion to the effective condition number when the condition number is smaller than 10^{16}.

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