COMMUNICATIONS IN NUMERICAL METHODS IN ENGINEERING
Commun. Numer. Meth. Engng (2009)
Published online in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/cnm.1275

Investigation of regularized techniques for boundary knot method

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SUMMARY

This study investigates regularization techniques for the boundary knot method (BKM). We consider three regularization methods and two approaches for the determination of the regularization parameter. Our numerical experiments show that Tikhonov regularization in conjunction with generalized cross-validation approach outperforms the other regularization techniques in the BKM solution of Helmholtz and modified Helmholtz problems. Copyright © 2009 John Wiley & Sons, Ltd.

Received 16 February 2009; Revised 27 April 2009; Accepted 28 April 2009

KEY WORDS: boundary knot method; regularization method; singular value decomposition; Helmholtz problem

1. INTRODUCTION

Recent years have witnessed a research boom in boundary meshless methods, such as the method of fundamental solutions (MFS) [1, 2], boundary knot method (BKM) [3, 4], boundary collocation method [5, 6], boundary node method [7, 8], and modified MFS [9–11] etc. In particular, the BKM is found to produce very accurate solution of the Helmholtz and modified Helmholtz problems. However, the convergence curves of this method are often oscillatory when using a large number of knots, which is also encountered in the other global collocation method such as the MFS. The reason for this phenomenon may contribute to the severely ill-conditioned full interpolation matrix.

In order to remedy this troublesome ill-conditioned problem, the regularization technique has been investigated on its utility to improve the accuracy of the global collocation boundary methods. For instance, Wei *et al.* [12] makes a comprehensive comparison of various regularization techniques in the MFS solution of inverse Cauchy problems. Ramachandran [13] uses the singular value decomposition (SVD) to resolve the ill-conditioning of the MFS discretization algebraic equations,

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Contract/grant sponsor: National Natural Science Foundation of China; contract/grant number: 10672051

and his conclusions are that direct solution of the MFS equations by Gaussian elimination are unreliable in some cases and that the SVD can be used to overcome this drawback. However, Chen *et al.* [14] re-examine the results given in [13] and argue that the SVD is not necessary in the MFS solution of direct problems. It is noted that the truncated singular value decomposition (TSVD) is clearly superior to Gaussian elimination for noisy boundary conditions [14]. On the other hand, the TSVD is also employed in the BKM solution of inverse problems [15, 16]. All these studies, however, have mainly focused on the solution accuracy rather than on the solution stability without a detailed investigation on the convergence behaviors. To our best knowledge, the regularization technique has also never been examined on the BKM stability in the solution of direct problems.

Motivated by the work mentioned above, this study investigates three regularization techniques and two approaches in choosing regularization parameters in the BKM solution of Helmholtz equations. The BKM is employed to discretize the equation. And then, to obtain a stable numerical scheme, regularization methods are used in solving the resulting discretized algebraic equations. Numerical experiments exhibit that the BKM coupled with Tikhonov regularization (TR) using generalized cross-validation (GCV) regularization parameter performs best in terms of stability for solving direct problems of Helmholtz and modified Helmholtz equations.

2. FORMULATION OF BKM

For simplicity, we consider solving well-posed boundary value problems for the Helmholtz equation:

$$\nabla^2 u+\lambda^2 u=0 \quad \text{in } \Omega \tag{1}$$

$$u(x)=\bar{u}(x) \quad \text{on } \Gamma_D \tag{2}$$

$$\frac{\partial u}{\partial n}=\bar{q}(x) \quad \text{on } \Gamma_N \tag{3}$$

where $\bar{u}(x)$ and $\bar{q}(x)$ are the known functions, Ω denotes the solution domain in $\mathbb{R}^d$ and $\partial\Omega(=\Gamma_D\cup\Gamma_N)$ its boundary, where d stands for the dimensionality of the space and n represents the unit outward normal.

In the case that λ is purely imaginary, the modified Helmholtz equation that has the similar form to Equation (1) is given by

$$\nabla^2 u-\lambda^2 u=0 \quad \text{in } \Omega \tag{4}$$

The non-singular general solution of the homogeneous Helmholtz equation (1) and homogeneous modified Helmholtz equation (4) are, respectively, given by

$$u_n^*(r)=\left(\frac{\lambda}{2\pi r}\right)^{(n/2)-1} J_{(n/2)-1}(\lambda r), \quad n\geqslant 2 \tag{5}$$

and

$$u_n^*(r)=\frac{1}{2\pi}\left(\frac{\lambda}{2\pi r}\right)^{(n/2)-1} I_{(n/2)-1}(\lambda r), \quad n\geqslant 2 \tag{6}$$

DOI: 10.1002/cnm

where J denotes the Bessel function of the first kind and I stands for the modified Bessel functions of the first kind, r represents the Euclidean norm distance. Since there is no singularity in (5) or (6), all collocation knots are placed on physical boundary and can be used as either source or response points.

By using the non-singular general solution (5) or (6), the solution of Equation (1) or Equation (4) can be approximated by

$$u(x_i)=\sum_{j=1}^{N}\alpha_j u_n^*(r_{ij}) \tag{7}$$

where j is index of source points on physical boundary, N denotes the total number of boundary knots, α_j the unknown coefficients and $r_{ij}=\sqrt{(x_i-x_j^2)+(y_i-y_j)^2}$, where i stands for index of collocation points on physical boundary. By collocating boundary Equations (2) and (3), we have

$$\sum_{j=1}^{N}\alpha_j u_n^*(r_{ij})=\bar{u}(x_i),\quad x_i\in\Gamma_D \tag{8}$$

$$\sum_{j=1}^{N}\alpha_j \frac{\partial u_n^*(r_{kj})}{\partial n}=\bar{q}(x_k),\quad x_k\in\Gamma_N \tag{9}$$

Equations (8)–(9) can be written in the following matrix system:

$$A\alpha=b \tag{10}$$

where $A=(A_{ij})$ is an interpolation matrix and $\alpha=(\alpha_1,\alpha_2,\ldots,\alpha_n)^{\mathrm{T}}$. We notice that, due to the global interpolation approach, the BKM produces a highly ill-conditioned and dense matrix system when a large number of boundary knots are used. For more details, we refer readers to References [3, 4].

An interesting and significant aspect of discrete ill-posed problems is that the ill-conditioning of a given problem does not prevent us from getting meaningful approximate solutions. Rather, it implies that the standard methods in numerical linear algebra for solving Equation (10), such as Gaussian elimination, may not be suitable for solving this type of problems. As such, regularization methods are proposed to alleviate the difficulty of highly ill-conditioning problems [17–20]. We briefly introduce some of them in the following section.

3. REGULARIZATION METHODS

Before presenting our numerical results, we give a brief discussion of some regularization methods.

3.1. Singular value decomposition (*SVD*)

As is well known, the matrix A in Equation (10) can be decomposed as [13]

$$A=\mathrm{UDV}^{\mathrm{T}} \tag{11}$$

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where $U=[u_1, u_2, \ldots, u_N]$ and $V=[v_1, v_2, \ldots, v_N]$ are matrices with orthogonal columns, $U^{\mathrm{T}}U = V^{\mathrm{T}}V = I_N$, the superscript $^{\mathrm{T}}$ represents the transpose of a matrix, I_N denotes the identity matrix, and D is a diagonal matrix with diagonal elements

$$\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_N \geqslant 0 \tag{12}$$

where σ_i, $1 \leqslant i \leqslant N$, are called the singular values of A while the vectors u_i and v_i are the left and right singular vectors of A, respectively.

Using Equation (11), we can solve Equation (10) in the following form:

$$\alpha = \sum_{i=1}^{N} \frac{u_i^{\mathrm{T}} b}{\sigma_i} v_i \tag{13}$$

We note that the ill-conditioning of A is due to the small singular values as shown in the denominator of (13). Based on the SVD, we present some commonly used regularization methods for ill-posed problems in the following subsection.

3.2. Regularization methods for discrete problems

The three most widely used regularization methods are the TSVD, TR method and damped singular value decomposition (DSVD).

In order to show the completeness of this paper, concise explanation on these methods is given as follows:

TSVD method: To obtain a better estimate of the least-squares solution, the TSVD solution is often used. It is given by approximating a rank$-N$ full matrix A by a rank K matrix in which only the largest K singular values are retained.

$$A_K = \sum_{i=1}^{K} u_i \sigma_i v_i^{\mathrm{T}} \tag{14}$$

In this way, matrix A in Equation (11) is replaced by A_K, which has a well-defined null space of dimension $N-K$ spanned by the right singular value vectors, $v_{K+1}, \ldots, v_N$. The original linear system Equation (11) is then replaced by the following problem set of Equation (15), where b is ideal noise-free data obtained at the minimized point. The resulting TSVD solution of Equation (15) is given by α_K and Equation (16).

$$\min \|\alpha\|_2 \quad \text{is subject to} \quad \min \|A_K \alpha - b\|_2 = \min \tag{15}$$

$$\alpha_K = \sum_{i=1}^{K} \frac{u_i^{\mathrm{T}} b}{\sigma_i} v_i \tag{16}$$

where $K \leqslant N$ is also a regularization parameter.

TR method: One of the most popular regularization methods is the TR, which in its simplest form replaces the linear system (10) by the minimization problem

$$\min_{\alpha \in R^n} \|A\alpha - b\|^2 + \mu^2 \|\alpha\|^2 \tag{17}$$

Here $\mu \geqslant 0$ is a regularization parameter. Throughout this paper $\|.\|$ denotes the Euclidean norm.

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The Tikhonov-regularized technique based on SVD can then be expressed as

$$\alpha_\mu = \alpha_{\min} = \sum_{i=1}^{l} f_i \frac{u_i^{\mathrm{T}} b}{\sigma_i} v_i \tag{18}$$

where the Wiener weights are

$$f_i = \frac{\sigma_i^2}{\sigma_i^2 + \mu^2} \tag{19}$$

and l is the rank of A.

DSVD method: A less known regularization method that is based on SVD is the DSVD. Here, instead of using the filter factors (19) in the TR, one introduces a smoother cut-off by means of filter factors f_i defined as

$$f_i = \frac{\sigma_i}{\sigma_i + \mu} \tag{20}$$

These filter factors decay slower than the Tikhonov filter factors and thus, in a sense, introduces less filtering.

The suitable value of the regularization parameter $\mu \geqslant 0$ is chosen by the L-curve criterion (LC) and the GCV in this paper.

3.3. Regularization parameters

The determination of a satisfactory value for the regularization parameter μ is crucial and is still under intensive research [20]. In this paper, we use the LC criterion and the GCV to choose a good regularization parameter.

LC for choosing the regularization parameter [17, 21]: A proper choice of the regularization parameter μ is essential in the successful use of a regularization method. Define a curve

$$L := \{(\log\|\alpha_\mu\|, \log\|A\alpha_\mu - b\|) : \mu \geqslant 0\} \tag{21}$$

The above curve is referred to as the L-curve, because it is shaped like the letter L for a large class of problems. We note here that the L-curve is a continuous curve when the regularization parameter is real in the TR and the DSVD. In numerical computation, the point with maximum curvature will be searched as the corner of the L-curve. For the regularization methods with a discrete regularization parameter, such as in TSVD, a finite set of points

$$\{(\log\|\alpha_q\|, \log\|A\alpha_q - b\|) : q = 1, 2, \ldots, N\} \tag{22}$$

will be obtained and interpolated by a spline curve. The point on the spline curve with the maximum curvature is then chosen as the desirable regularization parameter.

The L-curve is very attractive because the method shows how the regularized solution changes with the regularization parameter μ.

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GCV for choosing the regularization parameter [12]: The GCV is a statistical method that estimates the optimal value of the regularization parameter, by minimizing the functional

$$V(K)=\frac{\frac{1}{N}\|(I-A(K))b\|^2}{\left[\frac{1}{N}\mathrm{trace}(I-A(K))\right]^2} \tag{23}$$

The influence matrix $A(K)$ is defined as follows:

$$A\alpha_K = A(K)b \tag{24}$$

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

$$T(K)=\tfrac{1}{N}\|A(\alpha_K-\alpha)\|^2 \tag{25}$$

In the following section, as a comparison to the BKM with no regularization technique, numerical results are given by using the BKM coupled with six regularized methods: GCV-TR, LC-TR, GCV-DSVD, LC-DSVD, GCV-TSVD and LC-TSVD.

4. NUMERICAL RESULTS AND DISCUSSIONS

To examine the accuracy and stability of the proposed regularization methods given in the above sections, we test four benchmark cases of homogeneous Helmholtz and modified Helmholtz problems. The relative average error (root mean-square relative error: RMSE) in the following figures is defined as follows:

$$\mathrm{RMSE}=\sqrt{\frac{1}{N}\sum_{j=1}^{N}\left|\frac{u(x_j)-\tilde{u}(x_j)}{u(x_j)}\right|^2}$$

for $|u(x_j)|\geqslant 10^{-3}$ and

$$\mathrm{RMSE}=\sqrt{\frac{1}{N}\sum_{j=1}^{N}|u(x_j)-\tilde{u}(x_j)|^2}$$

for $|u(x_j)|<10^{-3}$, where j is the index of inner point we are interested in, $u(x_j)$ and $\tilde{u}(x_j)$ the exact and numerical solutions, respectively, and N denotes the total number of interior testing knots. The convergence behavior of the BKM using six regularized methods are shown in the given curves of the relative average error versus the number of boundary knots. MATLAB regularization code developed by Hansen [18] has been used in our computations.

4.1. Case 1: elliptic domain case

Here, we consider the Dirichlet homogeneous Helmholtz equation on an elliptic domain

$$\nabla^2 u(x,y)+u(x,y)=0, \quad (x,y)\in\Omega \tag{26}$$

$$u(x,y)=\sin(x)\sinh(x)+\cos(y), \quad (x,y)\in\partial\Omega \tag{27}$$

where $\Omega=\{(x,y):x^2/4+y^2=1\}$.

DOI: 10.1002/cnm

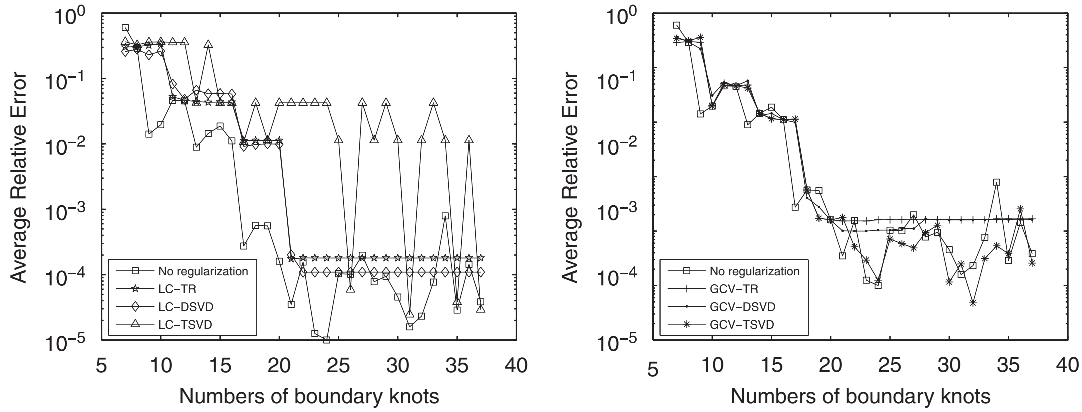

Figure 1. Relative average error curves for Case 1.

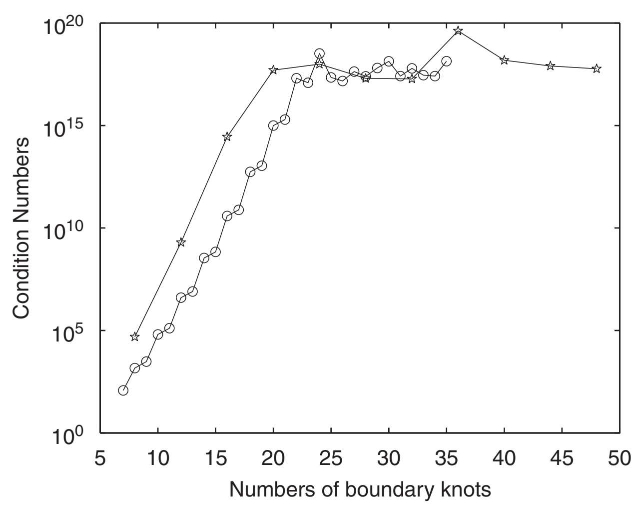

Figure 2. Condition number curves for Helmholtz problems with elliptic '○' and modified Helmholtz problems with rectangular domains '⋆'.

From Figure 1, we notice that convergence curve of the BKM without regularization techniques is quite oscillatory when the number of boundary knots becomes large. With using either DSVD or TR under the regularization parameter LC or GCV, the BKM solution accuracy degrades by one order of magnitude, but either BKM convergence curve appears far more stable. On the other hand, the LC-DSVD fails to yield reasonable BKM solution in this case.

Corresponding to Figure 1, Figure 2 shows the condition number variation curves versus the number of boundary knots, from which we can see a sharp increase in the condition number as a small number of boundary knots are added. This may partially explain the oscillatory behaviors of convergence curves illustrated in Figure 1.

DOI: 10.1002/cnm

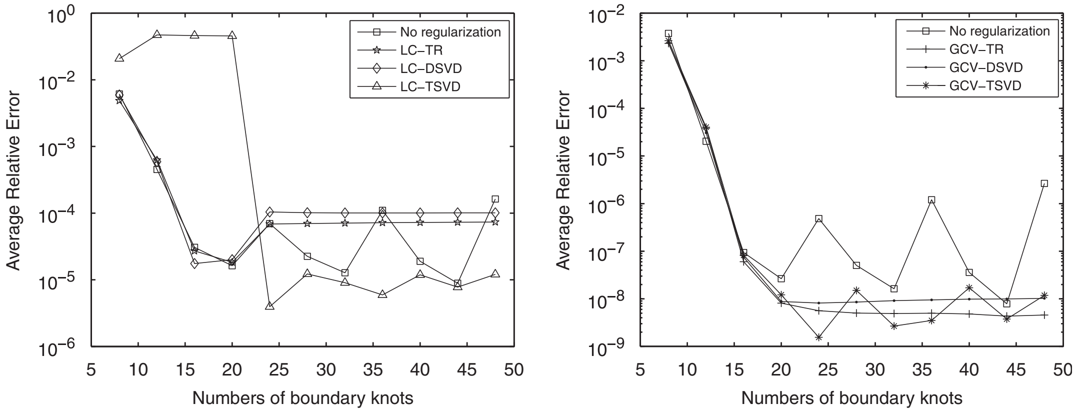

Figure 3. Relative average error curves for Case 2.

4.2. Case 2: *square domain case*

In this case, we examine the modified Helmholtz problem on a unit square domain with two Dirichlet edges $(x=1, y=1)$ and two Neumann edges $(x=0, y=0)$. The analytical solution is given by

$$u(x, y) = \mathrm{e}^{(x+y)} \tag{28}$$

The wave number of the non-singular general solution (5) is $\lambda=\sqrt{2}$ [4]. The curve of relative average error against the number of boundary knots is plotted in Figure 3. It is noted that the BKM with no regularization technique still encounters distinct oscillation. We can also see from Figure 3 that GCV-TR exhibits smooth convergence curve, and the BKM solution accuracy of GCV-TR is even higher than the one with no regularization technique. Corresponding to Figure 3, condition number curve in Figure 2 illustrates highly ill-conditioning nature of the influence matrices.

4.3. Case 3: *triangular domain case*

We consider Helmholtz problems with high wave numbers in this case. The boundary knots are uniformly distributed on an equilateral triangle domain with the left corner at the coordinate origin and side length 4. The Helmholtz problem of a high wave number $\lambda=100$ with mixed boundary conditions (Neumann edges the bottom side $x=0$ and others Dirichlet boundary) is considered. The analytical solution is given by

$$u(x, y) = \sin(\lambda x) + \cos(\lambda y) \tag{29}$$

In Figure 4, condition number curve is again shown versus the number of boundary knots in a highly increasingly rate. As shown in Figure 5, the relative average error curves of GCV-TR and GCV-DSVD work very well, but LC-TSVD fails to give an acceptable numerical result for this problem. The BKM with no regularization technique also has the oscillatory problem.

DOI: 10.1002/cnm

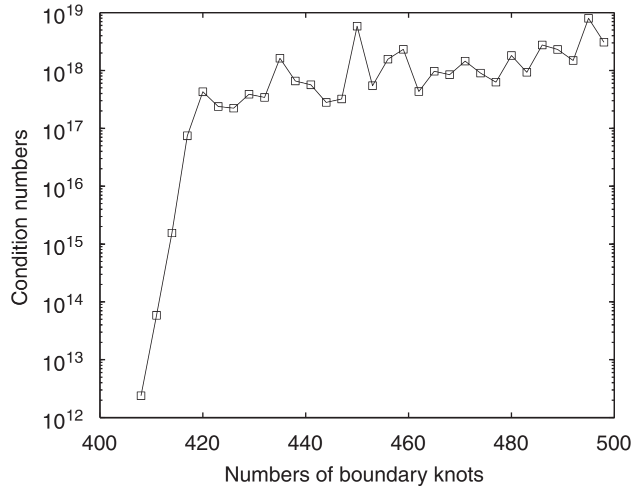

Figure 4. Configuration of condition number curve for Case 3.

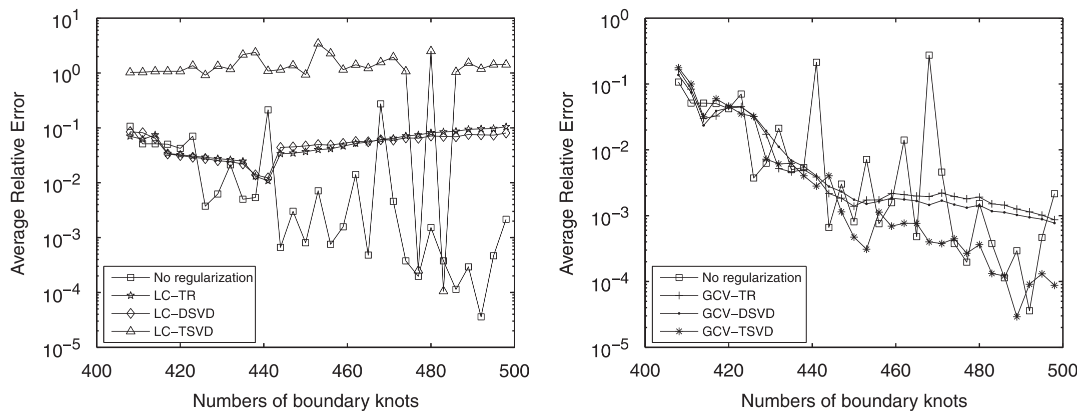

Figure 5. Relative average error curves for Case 3.

4.4. *Case 4*: *irregular domain case*

Next we consider a complex-shaped geometric case, as sketched in Figure 6, which involves mixed boundary conditions, namely, two adjacent Neumann edges ($x=0, y=0$) and the rest Dirichlet edge. The analytical solution for Helmholtz problem is given as

$$u(x, y) = \sin(x)\cos(y) \tag{30}$$

with wave number $\lambda = \sqrt{2}$. The condition number curve for this case is shown in Figure 7. Relative average error curves versus the number of boundary knots are shown in Figure 8, from which robust curves are shown by TR or DSVD using LC or GCV. The accuracy of GCV-TR and GCV-DSVD are even higher than the BKM with no regularization technique.

DOI: 10.1002/cnm

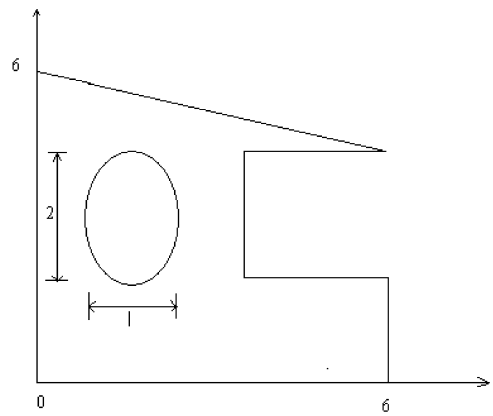

Figure 6. Configuration of 2D irregular domain.

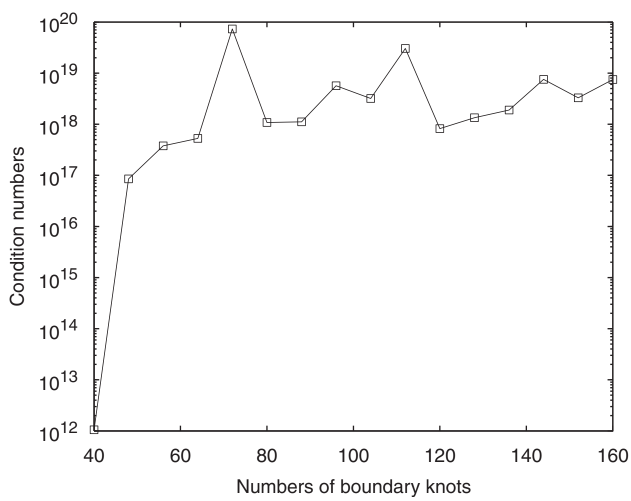

Figure 7. Configuration of condition number curve for Case 4.

4.5. *Discussions*

In terms of the convergence stability in the above-tested cases, we can conclude the numerical results in the following table:

	Regularization method		
Parameter	TSVD	TR	DSVD
LC	⋆	⋆⋆	⋆⋆
GCV	⋆⋆⋆⋆	⋆⋆⋆⋆⋆	⋆⋆⋆

Note: The convergence stability is scaled up from 1 to 5 '⋆'.

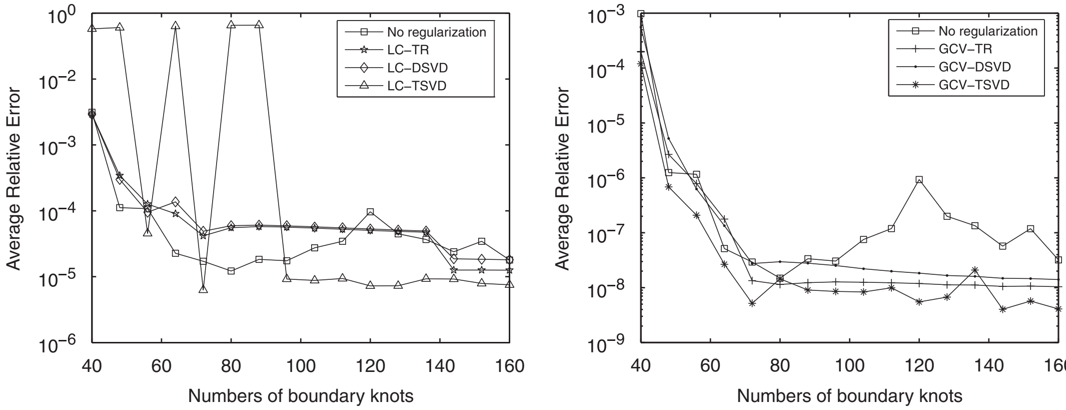

Figure 8. Relative average error curves for Case 4.

5. CONCLUDING REMARKS

Coupled with three regularization techniques and two algorithms for selecting regularization parameters, we are able to overcome the numerical instability induced from highly dense and ill-conditioned BKM interpolation matrix. In stark contrast, without an appropriate regularization, the direct use of the standard algebraic equation solvers, such as Gaussian elimination, often results in an oscillatory convergence curve when using a large number of boundary knots.

From the foregoing numerical results and discussions, we observe that the TR using GCV regularization parameters exhibits good performances for all tested problems in Section 4. Although TSVD using LC regularization technique is excellent for solving inverse problems with noisy boundary conditions, it fails to yield acceptable numerical approximation for all problems tested in this study.

ACKNOWLEDGEMENTS

We are very grateful of Prof. C.S. Chen for helpful suggestions to improve academic quality and readability of this paper. The work described in this paper was supported by a research project funded by the National Natural Science Foundation of China (Project No. 10672051).

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DOI: 10.1002/cnm