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Optimally Generalized Regularization Methods for Solving Linear Inverse Problems

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Abstract: In order to solve ill-posed linear inverse problems, we modify the Tikhonov regularization method by proposing three different preconditioners, such that the resultant linear systems are equivalent to the original one, without dropping out the regularized term on the right-hand side. As a consequence, *the new regularization methods can retain both the regularization effect and the accuracy of solution*. The preconditioned coefficient matrix is arranged to be **equilibrated** or **diagonally dominated** to derive the **optimal scales** in the introduced preconditioning matrix. Then we apply the iterative scheme to find the solution of ill-posed linear inverse problem. Two theorems are proved that the iterative sequences are monotonically convergent to the true solution. The presently proposed optimally generalized regularization methods are able to overcome the ill-posedness of linear inverse problems, and provide rather accurate numerical solution.

Keywords: Inverse Problem, Ill-posed linear system, Optimally generalized Tikhonov regularization method (OGTRM), Tikhonov regularization method (TRM), modified Tikhonov regularization method (MTRM), Generalized relaxed steepest descent method (GRSDM)

1 Introduction

In this paper we propose generalized and optimal Tikhonov regularization methods to solve the linear inverse problem, which might be recast to the following linear equations system:

$$\mathbf{V}\mathbf{x} = \mathbf{b}_1, \tag{1}$$

where $\det(\mathbf{V}) \neq 0$ and $\mathbf{V} \in \mathbb{R}^{n\times n}$ is an ill-conditioned, and generally unsymmetric matrix. Finding the solution of such an ill-posed linear system is an important issue

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for many linear inverse problems and numerical solutions of linear problems. In a practical situation of linear equations which arise in scientific problems, the data $\mathbf{b}_1$ are rarely given exactly; instead of, the noises in $\mathbf{b}_1$ are unavoidable due to the measurement error. Therefore, we may encounter the problem that the numerical solution of an ill-posed system of linear equations may deviate from the exact one to a great extent, when $\mathbf{V}$ is severely ill-conditioned and $\mathbf{b}_1$ is perturbed by noise.

Hansen (1992), and Hansen and O'Leary (1993) have explained that the Tikhonov regularization method [Tikhonov and Arsenin (1977)] to solve ill-posed linear problem is a trade-off between the size of the regularized solution and the quality to fit the given data:

$$\min_{\mathbf{x}\in\mathbb{R}^n} \varphi(\mathbf{x}) = \min_{\mathbf{x}\in\mathbb{R}^n} \left[\|\mathbf{V}\mathbf{x}-\mathbf{b}_1\|^2 + \alpha\|\mathbf{x}\|^2\right]. \tag{2}$$

To account for the sensitivity to noise, it is customary to use a "regularization" method to solve the ill-posed problem [Kunisch and Zou (1998); Wang and Xiao (2001); Xie and Zou (2002); Resmerita (2005)], wherein a suitable regularization parameter is used to seeking a better balance of the error of approximation and the propagated data error. Several regularization methods were developed to follow the pioneering work of Tikhonov and Arsenin (1977). For a large scale system, the main choice is the iterative regularization algorithm, which works if an early stopping criterion is used to prevent the introduction of noisy components into the approximate solutions.

Here, we briefly review four existent techniques to select the regularization parameter α used in Eq. (2), where as pointed out by Kilmer and O'Leary (2001) many of these algorithms are rather complicated.

(i) **The discrepancy principle** [Morozov (1966)] says that the regularization parameter should be chosen such that the norm of the residual vector corresponding to the regularized solution $\mathbf{x}_{\text{reg}}$ is $\tau\sigma$:

$$\|\mathbf{V}\mathbf{x}_{\text{reg}}-\mathbf{b}_1\| = \tau\sigma, \tag{3}$$

where $\tau > 1$ is some predetermined real number. Note that $\mathbf{x}_{\text{reg}} \longrightarrow \mathbf{x}_{\text{true}}$ if $\sigma \longrightarrow 0$.

(ii) **The generalized cross-validation** [Goloub, Heath and Wahba (1979)] does not depend on a priori information about the variance of noise σ. One finds the parameter α that minimizes the following GCV functional:

$$G(\alpha) = \frac{\|(\mathbf{I}_n - \mathbf{V}[\mathbf{V}^{\text{T}}\mathbf{V}+\alpha\mathbf{I}_n]^{-1}\mathbf{V}^{\text{T}})\mathbf{b}_1\|^2}{[\text{Trace}(\mathbf{I}_n - \mathbf{V}[\mathbf{V}^{\text{T}}\mathbf{V}+\alpha\mathbf{I}_n]^{-1}\mathbf{V}^{\text{T}})]^2}. \tag{4}$$

(iii) For **the *L*-curve**, the plot of the norm of $\mathbf{x}_{\text{reg}}$ versus the corresponding residual norm for each of a set of the regularization parameter values, was introduced by Hansen (1992). The best regularization parameter should lie on the corner of the *L*-curve, since for values higher than this, the residual norm increases without reducing the norm of $\mathbf{x}_{\text{reg}}$ much, while for values smaller than this, the norm $\|\mathbf{x}_{\text{reg}}\|$ increases rapidly without much decreasing the residual norm.

(iv) **The iteration technique** was introduced by Engl (1987) and Gfrerer (1987). Basically, they constructed an iterative sequence:

$$(\mathbf{V}^{\mathrm{T}}\mathbf{V}+\alpha\mathbf{I}_n)\mathbf{x}^{j}_{\alpha,\sigma}=\mathbf{b}+\alpha\mathbf{x}^{j-1}_{\alpha,\sigma},\quad j=1,\ldots,m, \tag{5}$$

where $\mathbf{b}=\mathbf{V}^{\mathrm{T}}\mathbf{b}_1$, by starting from the initial value of $\mathbf{x}^{0}_{\alpha,\sigma}=\mathbf{0}$, and then inserted the convergent solution of Eq. (5) into Eq. (3) to iteratively solve the implicit nonlinear algebraic equation for finding the best α.

In this paper we introduce simple modifications of the Tikhonov regularization method for solving the ill-posed linear inverse problem, where the regularization parameter α is no longer restricted to be a small number, because the novel regularization methods do not perturb the original ill-posed linear system. On the other hand, we no more need to pay much attention on the choice of the regularization parameter α.

Earlier on, the author and his coworkers have developed several methods to solve the ill-posed linear problems: using the fictitious time integration method as a filter for ill-posed linear system [Liu and Atluri (2009a)], a modified polynomial expansion method [Liu and Atluri (2009b)], the non-standard group-preserving scheme [Liu and Chang (2009)], a vector regularization method [Liu, Hong and Atluri (2010)], the preconditioners and postconditioners generated from a transformation matrix, obtained by Liu, Yeih and Atluri (2009) for solving the Laplace equation with a multiple-scale Trefftz basis functions, the relaxed steepest descent method [Liu (2011a, 2012a)], the optimal iterative algorithm [Liu and Atluri (2011a)], an optimally scaled vector regularization method [Liu (2012b)], an adaptive Tikhonov regularization method [Liu (2012c)], the best vector iterative method [Liu (2012d)], as well as a globally optimal iterative method [Liu (2012e)].

This paper is organized as follows. We first modify the Tikhonov regularization method by using the preconditioner and iteration for solving an ill-posed linear system in Section 2. In Section 3 we describe the optimally generalized Tikhonov regularization methods by using the preconditioner and iteration method, where the preconditioned matrix is optimized based on the concepts of equilibrated matrix and the diagonally dominated matrix, which are then compared with the generalized Tikhonov regularization method. The above methods require some inner iterations to solve the regularized linear systems. In Section 4 we introduce the third preconditioner and directly use an iterative scheme without inner iteration to solve the regularized linear system. In Section 5 we give numerical examples of the Hilbert linear system, backward heat conduction problem, and the inverse Cauchy problems to test the efficiency and accuracy of the novel iteratively regularized algorithms. Finally, the conclusions are drawn in Section 6.

2 An iterative Tikhonov regularization method

It is known that the original Tikhonov regularization method is solving the following regularized normal equation:

$$(\mathbf{V}^{\mathrm{T}}\mathbf{V}+\alpha\mathbf{I}_n)\mathbf{x}=\mathbf{b}, \tag{6}$$

which is obtained from Eq. (2), where $\mathbf{b} := \mathbf{V}^{\mathrm{T}}\mathbf{b}_1$, and α is a regularization parameter to be determined. Several methods have been introduced in Section 1 to find the best value of α. However, we need to emphasize that the Tikhonov regularization method perturbs the original system into a new one by adding a perturbed term $\alpha\mathbf{x}$ on the left-hand side, which plays the role of regularization to stabilize the coefficient matrix $\mathbf{V}^{\mathrm{T}}\mathbf{V}+\alpha\mathbf{I}_n$. So the regularization parameter α must be a suitable number, and is small enough to make a little perturbation of the original equation.

Let us begin with the following preconditioner:

$$\mathbf{P}_1 := \mathbf{V}^{\mathrm{T}}+\alpha\mathbf{V}^{-1}, \tag{7}$$

where $\mathbf{V}^{-1}$ is the inversion of $\mathbf{V}$, which exists due to the assumption of $\det(\mathbf{V}) \neq 0$. Applying $\mathbf{P}_1$ to Eq. (1) and using that equation again, we have

$$\begin{aligned}
&(\mathbf{V}^{\mathrm{T}}+\alpha\mathbf{V}^{-1})\mathbf{V}\mathbf{x}=(\mathbf{V}^{\mathrm{T}}+\alpha\mathbf{V}^{-1})\mathbf{b}_1,\\
&(\mathbf{V}^{\mathrm{T}}\mathbf{V}+\alpha\mathbf{I}_n)\mathbf{x}=\mathbf{b}+\alpha\mathbf{V}^{-1}\mathbf{b}_1,\\
&(\mathbf{V}^{\mathrm{T}}\mathbf{V}+\alpha\mathbf{I}_n)\mathbf{x}=\mathbf{b}+\alpha\mathbf{x}.
\end{aligned} \tag{8}$$

It is interesting that the regularized Eq. (8) bears certain similarity with the Tikhonov regularization equation (6); but here the regularization term $\alpha\mathbf{x}$, not only appears on the left-hand side, but also on the right-hand side, which is different from that in Eq. (6), where the regularization term $\alpha\mathbf{x}$ is dropped out from the right-hand side.

However, in its present form, Eq. (8) can do nothing, which is just equivalent to the normal form of the original equation (1). However, we can consider an iterative process to find the solution of $\mathbf{x}$ by

$$\mathbf{A}\mathbf{x}_{k+1}=\mathbf{b}+\alpha\mathbf{x}_k, \tag{9}$$

where

$$\mathbf{A} := \mathbf{V}^{\mathrm{T}}\mathbf{V} + \alpha \mathbf{I}_n. \tag{10}$$

Starting from $\mathbf{x}_0 = \mathbf{0}$ we can apply the conjugate gradient method (CGM) to solve the above linear system and generate a sequence of vectors $\mathbf{x}_k$, $k = 1, \ldots, m$. In each inner iteration we apply the CGM to solve the linear system (9) under a convergence criterion specified by a value ε_1. When the following convergence criterion is satisfied $\|\mathbf{x}_{k+1} - \mathbf{x}_k\| \leq \varepsilon_2$, we also stop the outer iterative sequence, and then the solution of $\mathbf{x}$ is obtained.

Theorem 1: *For Eq. (9) with $\alpha > 0$ the iterative sequence $\mathbf{x}_k$ converges to the true solution $\mathbf{x}_{true}$ monotonically.*

Proof: Let

$$\varepsilon_k = \mathbf{x}_k - \mathbf{x}_{k-1}, \; \varepsilon_{k+1} = \mathbf{x}_{k+1} - \mathbf{x}_k \tag{11}$$

be two consecutive relative vectorial errors of the iterative solutions. From Eq. (9) it follows that

$$\begin{aligned} \mathbf{A}\mathbf{x}_k &= \mathbf{b} + \alpha \mathbf{x}_{k-1}, \\ \mathbf{A}\mathbf{x}_{k+1} &= \mathbf{b} + \alpha \mathbf{x}_k, \end{aligned} \tag{12}$$

from which by subtracting the first equation from the second equation and using Eq. (11) we can obtain

$$\mathbf{A}\varepsilon_{k+1} = \alpha \varepsilon_k. \tag{13}$$

It follows the following inequalities:

$$(\lambda_{\min} + \alpha)\|\varepsilon_{k+1}\| \leq \|\mathbf{A}\varepsilon_{k+1}\| = \alpha\|\varepsilon_k\|, \tag{14}$$

where $\lambda_{\min} > 0$ is the smallest eigenvalue of $\mathbf{V}^{\mathrm{T}}\mathbf{V}$. Hence we have

$$\|\varepsilon_{k+1}\| \leq \frac{\alpha}{\lambda_{\min} + \alpha}\|\varepsilon_k\|, \tag{15}$$

which is a monotonically decreasing sequence for the norm $\|\varepsilon_k\|$ of the relative vectorial error when $\alpha > 0$ and hence $\alpha/(\lambda_{\min} + \alpha) < 1$. Thus when $\|\varepsilon_k\|$ monotonically tends to zero, the iterative solution $\mathbf{x}_k$ converges to the true solution $\mathbf{x}_{\mathrm{true}}$ monotonically. This ends the proof. □

The present regularization method does not perturb the original system, but mathematically converts it to a new problem by iteratively solving a sequence of regularized linear systems, and thus the parameter α does not need to be a small number, which can be selected such that the condition number of $\mathbf{A} := \mathbf{V}^{\mathrm{T}}\mathbf{V} + \alpha \mathbf{I}_n$ is smaller than that of $\mathbf{V}^{\mathrm{T}}\mathbf{V}$. This new regularization method will be named the modified Tikhonov regularization method (MTRM), which can remedy the shortcoming of the original Tikhonov regularization method that there exists nothing on the right-hand side in Eq. (6) to balance the perturbation term of $\alpha\mathbf{x}$ on the left-hand side. Hence, in the original Tikhonov regularization method, if one over emphasizes the regularization effect, the accuracy of solution may lose to a great extent. The MTRM does not have such a drawback.

The present MTRM is also different from the iterative Tikhonov regularization method as introduced in Section 1 with the item (iv), which was developed by Engl (1987) and Gfrerer (1987). They solved Eq. (5) and inserted the convergent solution into Eq. (3) to iteratively solve the implicitly nonlinear algebraic equation for finding the best value of α. Although Eqs. (9) and (5) are the same, here we approach it by using the preconditioner method, and we do not use it to find the best α; instead of, we directly use Eq. (9) to find the approximate solution $\mathbf{x}_k$, and α in Eq. (9) can be a quite large number, without restricting to be a small parameter.

3 Optimally generalized Tikhonov regularization method

A generalization of Eq. (2) can be written as

$$\min_{\mathbf{x}\in\mathbb{R}^n} \varphi(\mathbf{x}) = \min_{\mathbf{x}\in\mathbb{R}^n} \left[\|\mathbf{V}\mathbf{x} - \mathbf{b}_1\|^2 + \mathbf{x}^{\mathrm{T}}\mathbf{R}\mathbf{x} \right], \tag{16}$$

where $\mathbf{R}$ is a positive definite matrix. In the present study we only consider $\mathbf{R} := \mathrm{diag}(R_1, \ldots, R_n)$, where $R_k,\ k = 1, \ldots, n$ are positive real numbers, which will be optimized below.

3.1 The second preconditioner

Consider the second preconditioner to be

$$\mathbf{P}_2 := \mathbf{V}^{\mathrm{T}} + \mathbf{R}\mathbf{V}^{-1}, \tag{17}$$

and applying it to Eq. (1) and using that equation again, we have

$$
\begin{aligned}
&(\mathbf{V}^{\mathrm{T}}+\mathbf{R}\mathbf{V}^{-1})\mathbf{V}\mathbf{x}=(\mathbf{V}^{\mathrm{T}}+\mathbf{R}\mathbf{V}^{-1})\mathbf{b}_1,\\
&(\mathbf{V}^{\mathrm{T}}\mathbf{V}+\mathbf{R})\mathbf{x}=\mathbf{b}+\mathbf{R}\mathbf{V}^{-1}\mathbf{b}_1,\\
&(\mathbf{V}^{\mathrm{T}}\mathbf{V}+\mathbf{R})\mathbf{x}=\mathbf{b}+\mathbf{R}\mathbf{x}.
\end{aligned} \tag{18}
$$

By dropping out the regularized term $\mathbf{Rx}$ on the rigth-hand side we can recover to the form in Eq. (16). In this sense we have made an improvement of the generalized Tikhonov regularization method.

From the regularized linear system (**??**) we can derive an iterative process to find the unknown vector $\mathbf{x}$ by

$$\mathbf{A}\mathbf{x}_{k+1}=\mathbf{b}+\mathbf{R}\mathbf{x}_k, \tag{19}$$

where

$$\mathbf{A}:=\mathbf{V}^{\mathrm{T}}\mathbf{V}+\mathbf{R}. \tag{20}$$

Starting from $\mathbf{x}_0=\mathbf{0}$ we can apply the CGM to solve the above regularized linear system (19) and generate a sequence of vectors $\mathbf{x}_k$, $k=1,\ldots,m$. When the following convergence criterion is satisfied $\|\mathbf{x}_{k+1}-\mathbf{x}_k\|\leq\varepsilon_2$, we stop the outer iterative sequence, and meanwhile the solution of $\mathbf{x}$ is obtained.

Theorem 2: *For Eq. (19) with positive definite* $\mathbf{R}$ *the iterative sequence* $\mathbf{x}_k$ *converges to the true solution* $\mathbf{x}_{true}$ *monotonically.*

Proof: As that done in the proof of Theorem 1 we can derive

$$\mathbf{A}\varepsilon_{k+1}=\mathbf{R}\varepsilon_k. \tag{21}$$

Because $\mathbf{R}$ is positive definite, by Eq. (20) the following inequality holds:

$$\mathbf{A}\geq\lambda_{\min}\mathbf{I}_n+\mathbf{R}, \tag{22}$$

where $\lambda_{\min}>0$ is the smallest eigenvalue of $\mathbf{V}^{\mathrm{T}}\mathbf{V}$. From Eq. (21) it follows that

$$\|\mathbf{A}\varepsilon_{k+1}\|=\|\mathbf{R}\varepsilon_k\|, \tag{23}$$

Hence, from Eqs. (22) and (23) we have

$$\|\lambda_{\min}\mathbf{I}_n+\mathbf{R}\|\|\varepsilon_{k+1}\|\leq\|\mathbf{R}\|\|\varepsilon_k\|, \tag{24}$$

where the norm of a matrix is induced by the Euclidean norm of a vector. Due to $\lambda_{\min} > 0$ and $\mathbf{R}$ being positive definite the factor γ satisfies the following inequality:

$$\gamma := \frac{\|\mathbf{R}\|}{\|\lambda_{\min}\mathbf{I}_n + \mathbf{R}\|} < 1. \tag{25}$$

Hence, one has

$$\|\varepsilon_{k+1}\| \leq \gamma\|\varepsilon_k\|, \ \gamma < 1. \tag{26}$$

It is a monotonically decreasing sequence for the norm $\|\varepsilon_k\|$ of the relative vectorial error. Thus when $\|\varepsilon_k\|$ monotonically tends to zero, the iterative solution $\mathbf{x}_k$ converges to the true solution $\mathbf{x}_{\text{true}}$ monotonically. This ends the proof. □

3.2 The optimally scaled R_k

Now, the problem is how to choose the multiple-scale $R_k, \ k = 1,\ldots,n$ appeared in $\mathbf{R}$. Usually, the linear system (19) is severely ill-conditioned, and if we do not properly choose $\mathbf{R}$, the situation may become worse. So we have to look for values of $R_k, \ k = 1,\ldots,n$ which will render the linear system (19) to be less ill-conditioned. The problem becomes to search for the suitable scales $R_k, \ k = 1,\ldots,n$, such that the condition number of $\mathbf{A}$ is reduced as much as possible. Theoretically, there are theories of optimal scaling proposed by Bauer (1963), van der Sluis (1969), Gautschi (2011), and Liu (2012b, 2012f). A matrix is said to be **equilibrated** if all its rows or columns have the same norm, and under this condition the matrix is best conditioned. According to the idea of "equilibrated matrix", we can choose R_k, such that each row of the matrix $\mathbf{A}$ in Eq. (19) has the same Euclidean norm, say $R_0 > 0$, i.e.,

$$\sum_{k=1}^{n} A_{1k}^2 = \ldots = \sum_{k=1}^{n} A_{nk}^2 = R_0^2, \tag{27}$$

where A_{ij} denotes the ij-th component of $\mathbf{A}$. The constant R_0 can be selected by

$$R_0 \geq R_{\max} := \max_{i=1,\ldots,n} \sqrt{\sum_{k=1}^{n} C_{ik}^2}, \tag{28}$$

where C_{ik} denote the components of $\mathbf{C} := \mathbf{V}^{\mathrm{T}}\mathbf{V}$. Definitely, we can take

$$R_0 = R_{\max} + c_0, \tag{29}$$

where c_0 is a non-negative constant, whose value is problem dependent. Then, from Eqs. (20) and (27) through some manipulations we can derive

$$R_k = \beta \left(\sqrt{C_{kk}^2 + R_0^2 - \sum_{j=1}^{n} C_{kj}^2} - C_{kk} \right). \tag{30}$$

Here β is a stability factor to guarantee that the iterative process can converge fast.

On the other hand, we can require that the new coefficient matrix $\mathbf{A}$ has the same diagonal value R_0 like as a **diagonally dominated** matrix, such that we can derive

$$R_k = \beta(R_0 - C_{kk}), \tag{31}$$

where

$$R_0 = \max_{i=1,\ldots,n} C_{ii} + c_0, \tag{32}$$

and similarly β is a stability factor, and c_0 is a non-negative constant specified by the user.

For convenience we may call the present regularization method to be the *optimally generalized Tikhonov regularization method*: OGTRM(1), if Eq. (30) is used to select $R_k,\ k = 1,\ldots,n$, and the regularized linear system (19) is used to iteratively solve the unknown vector $\mathbf{x}$; alternatively, the OGTRM(2), if Eq. (31) is used to select $R_k,\ k = 1,\ldots,n$, and the regularized linear system (19) is used to iteratively solve the unknown vector $\mathbf{x}$. The present regularization methods do not perturb the original system, but mathematically convert it to a new problem by iteratively solving a sequence of regularized linear systems in Eq. (19).

4 A generalized relaxed steepest descent method

Let us further consider the third preconditioner:

$$\mathbf{P}_3 := \mathbf{V}^{\mathrm{T}} - \mathbf{E}^{-1}\mathbf{V}^{-1}, \tag{33}$$

and applying it to Eq. (1) we can derive

$$(\mathbf{V}^{\mathrm{T}}\mathbf{V} - \mathbf{E}^{-1})\mathbf{x} = \mathbf{b} - \mathbf{E}^{-1}\mathbf{x}, \tag{34}$$

where $\mathbf{E}$ is a positive definite matrix.

Instead of Eq. (19) to solve a linear system at each inner iterative loop, here we employ a directly iterative scheme to find the solution of $\mathbf{x}$ by

$$(\mathbf{V}^{\mathrm{T}}\mathbf{V} - \mathbf{E}^{-1})\mathbf{x}_k = \mathbf{b} - \mathbf{E}^{-1}\mathbf{x}_{k+1}, \tag{35}$$

which is obtained from Eq. (34). Thus through some operations we can derive

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{E}\mathbf{r}_k, \tag{36}$$

where

$$\mathbf{r}_k = \mathbf{b} - \mathbf{C}\mathbf{x}_k \tag{37}$$

is a residual vector for the normal equation:

$$\mathbf{C}\mathbf{x} = \mathbf{b}, \tag{38}$$

in which

$$\mathbf{C} := \mathbf{V}^{\mathrm{T}}\mathbf{V}, \tag{39}$$
$$\mathbf{b} := \mathbf{V}^{\mathrm{T}}\mathbf{b}_1. \tag{40}$$

The scheme in Eq. (36) is more time saving, which does not need an inner iteration. Upon letting

$$\mathbf{E} = (1-\gamma)\frac{\mathbf{r}_k^{\mathrm{T}}\mathbf{G}\mathbf{r}_k}{\mathbf{r}_k^{\mathrm{T}}\mathbf{G}\mathbf{C}\mathbf{G}\mathbf{r}_k}\mathbf{G} \tag{41}$$

in Eq. (36), we can derive the following algorithm (see the Appendix):
(i) Select a suitable value of $0 \leq \gamma < 1$, and assume an initial value of $\mathbf{x}_0$.
(ii) For $k = 0, 1, 2 \ldots$ we repeat the following iterations:

$$\mathbf{r}_k = \mathbf{b} - \mathbf{C}\mathbf{x}_k, \tag{42}$$
$$\mathbf{x}_{k+1} = \mathbf{x}_k + (1-\gamma)\frac{\mathbf{r}_k^{\mathrm{T}}\mathbf{G}\mathbf{r}_k}{\mathbf{r}_k^{\mathrm{T}}\mathbf{G}\mathbf{C}\mathbf{G}\mathbf{r}_k}\mathbf{G}\mathbf{r}_k. \tag{43}$$

If $\mathbf{x}_{k+1}$ converges according to a given stopping criterion $\|\mathbf{r}_{k+1}\| < \varepsilon_1$, then stop; otherwise, go to step (ii). The above parameter γ is a relaxed constant with $0 \leq \gamma < 1$. If we take $\mathbf{G} = \mathbf{I}_n$, then the above algorithm reduces to the relaxed steepest descent method [Liu (2011a, 2012a)]. If we take $\mathbf{G} = \mathbf{V}^{\mathrm{T}}\mathbf{V}$, or $\mathbf{G} = \mathbf{V}\mathbf{V}^{\mathrm{T}}$, we can obtain a different new algorithm. Hence, this algorithm is a generalized relaxed steepest descent method (GRSDM), with $\mathbf{G}$ being a positive definite matrix.

5 Numerical examples

5.1 Example 1: two simple but highly ill-conditioned linear systems

This example will illustrate that the present iterative regularization methods are better than the original Tikhonov regularization method. Before embarking on a further numerical test of the present methods, we give a simple example of the solution of a linear system of two linear algebraic equations:

$$\begin{bmatrix} 2 & 2 \\ 6 & 6.00001 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 4 \\ 12.00001 \end{bmatrix}. \tag{44}$$

The exact solution is $(x,y) = (1,1)$. We add a random noise $\sigma = 0.05$ on the data of $(4, 12.00001)^{\mathrm{T}}$, and apply the Tikhonov regularization method to solve this problem with $\alpha = 10^{-7}$, of which the solution is $(x,y) = (1.246, 0.754)$.

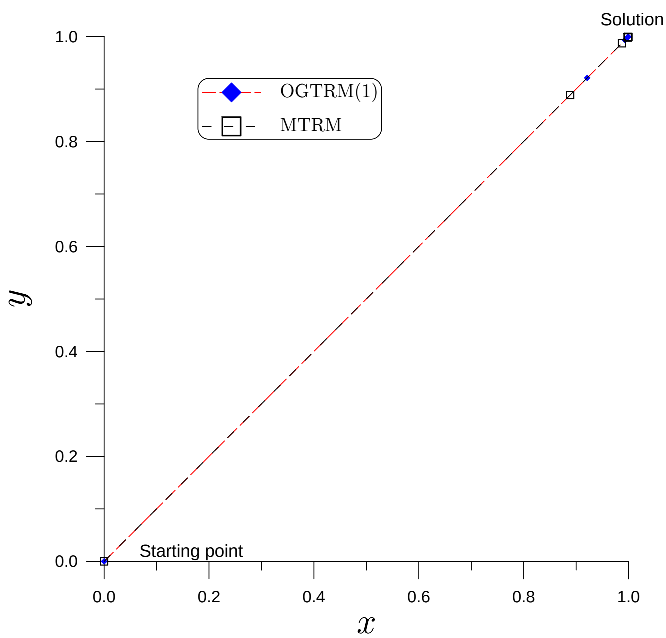

Figure 1: For example 1, comparing the iterative paths generated by the optimally generalized Tikhonov regularization method OGTRM(1), and the modified Tikhonov regularization method (MTRM).

We use the MTRM in Section 2 to solve this problem with $\alpha = 10$ (here, α is not necessary a small constant). It is interesting that the condition number is greatly reduced from $\text{Cond}(\mathbf{V}^{\text{T}}\mathbf{V}) = 1.59 \times 10^{13}$ to $\text{Cond}(\mathbf{V}^{\text{T}}\mathbf{V} + \alpha\mathbf{I}_n) = 9$, where $\mathbf{V}$ denotes the coefficient matrix in Eq. (44). A solution $(x,y) = (0.999611, 0.999613)$ is obtained, which is convergent with 15 iterations under the convergence criteria $\varepsilon_1 = 10^{-15}$ and $\varepsilon_2 = 10^{-3}$. The iterative path is shown in Fig. 1. Then, we use the OGTRM(1) in Section 3.2 to solve this problem with $c_0 = 5$ and $\beta = 1$. The condition number is greatly reduced to $\text{Cond}(\mathbf{V}^{\text{T}}\mathbf{V} + \mathbf{R}) = 12.75$. We obtain a solution of $(x,y) = (0.999582, 0.99960)$, which is convergent very fast with 12 iterations under the convergence criteria $\varepsilon_1 = 10^{-15}$ and $\varepsilon_2 = 10^{-3}$. The iterative path is compared with that obtained by the MTRM in Fig. 1. Although, the OGTRM(1) has obtained the solution with the same accuracy as that obtained by the MRTM, the OGTRM(1) converges faster than the MTRM. It can be seen that both the MTRM and OGTRM(1) are more accurate than the original Tikhonov regularization method with three orders. It is interesting that when we apply the GRSDM in Section 4 with $\mathbf{G} = \mathbf{C}$ and $\gamma = 0$ to solve the above linear system, it approaches to a very accurate solution $(x,y) = (0.99963, 0.99963)$ only through two iterations.

Next, in order to further test the new algorithm of GRSDM, we consider a more difficult linear system:

$$\begin{bmatrix} 2 & 6 \\ 2 & 6.0001 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 8 \\ 8.0001 \end{bmatrix}. \tag{45}$$

The condition number of this system is $\text{Cond}(\mathbf{V}^{\text{T}}\mathbf{V}) = 1.596 \times 10^{11}$, where $\mathbf{V}$ denotes the coefficient matrix . The exact solution is $(x,y) = (1,1)$. For this system the above algorithms MTRM and OGTRM are both not applicable.

Now we fix the noise to be $\sigma = 0.01$, $\varepsilon_1 = 10^{-8}$ and starting from an initial condition $(x_0, y_0) = (0.5, 0.5)$. By applying the Barzilai-Borwein method (BBM) [Barzilai and Borwein (1988)], it does not converge with 2000 iterations, and obtain an inaccurate solution of $(x,y) = (0.7, 1.1)$. Then we apply the RSDM algorithm [Liu (2011a)] with $\gamma = 0.2$ to this problem, which, through 2000 iterations, led to an approximate solution of $(x,y) = (1.004, 0.999)$ with the maximum error being 4.47×10^{-3}. When we apply the GRSDM with $\mathbf{G} = \mathbf{V}\mathbf{V}^{\text{T}}$ and $\gamma = 0$, it approaches to a very accurate solution $(x,y) = (1.00004, 1.00005)$ only through two iterations. Although, for a more ill-posed case with the above 6.0001 and 8.0001 replaced by 6.00001 and 8.00001, of which the condition number is raised to $\text{Cond}(\mathbf{V}^{\text{T}}\mathbf{V}) = 1.596 \times 10^{13}$, the GRSDM can also find the solution $(x,y) = (1.00005, 1.00005)$ only through two iterations.

5.2 Example 2: Hilbert linear equations system

The Hilbert matrix

$$V_{ij} = \frac{1}{i+j-1} \tag{46}$$

is notoriously ill-conditioned. It is known that the condition number of Hilbert matrix grows as $e^{3.5n}$ when n is very large. For the case with $n = 200$ the condition number is extremely huge to the order 10^{348}. The exact inverse of the Hilbert matrix has been derived by Choi (1983):

$$(\mathbf{V}^{-1})_{ij} = (-1)^{(i+j)}(i+j-1)\begin{pmatrix} n+i-1 \\ n-j \end{pmatrix}\begin{pmatrix} n+j-1 \\ n-i \end{pmatrix}\begin{pmatrix} i+j-2 \\ i-1 \end{pmatrix}^2. \tag{47}$$

Since the exact inverse has large integer entries when n is large, a small perturbation of the given data will be amplified greatly, such that the solution is contaminated seriously by errors. The program can compute the inverse by using the exact integer arithmetic for $n = 13$. Past that number the double precision approximation should be used. However, due to the overflow of arithmetic computation the inverse can be computed only for n which is much smaller than 200.

We apply the Tikhonov regularization method (TRM) with $\alpha = 10^{-4}$, the MTRM with $\alpha = 10^{-4}$, the OGTRM(1) with $c_0 = 0.5$ and $\beta = 1$, and the OGTRM(2) with $c_0 = 1$ and $\beta = 1$, to solve the linear equations system (1) with the Hilbert matrix as the coefficient matrix, where a random noise with an intensity $\sigma = 0.05$ is added on the input data on the right-hand side. The exact solutions are supposed to be $x_i = 1,\ i = 1,\dots,200$, and the absolute errors of numerical results are compared in Fig. 2(a), of which one can see that the present methods are more accurate than the Tikhonov regularization method. Both OGTRM(1) and OGTRM(2) are better than the MTRM and TRM. In Fig. 2(b) we show the norm of each column of the coefficient matrix $\mathbf{A}$ for the OGTRM(2). Even, we require that in the OGTRM(2) the diagonal elements have the same value, it also results in a quite better matrix near to the equilibrated matrix. This explains why the OGTRM(2) is the best one among the above four methods to solve this highly ill-posed linear problem with $n = 200$.

5.3 Example 3: backward heat conduction problem

When the backward heat conduction problem (BHCP) is considered in a spatial interval of $0 < x < \ell$ by subjecting to the boundary conditions at two ends of a slab:

$$u_t(x,t) = \kappa u_{xx}(x,t),\ \ 0 < t < T,\ \ 0 < x < \ell, \tag{48}$$

$$u(0,t) = u_0(t),\ \ u(\ell,t) = u_\ell(t), \tag{49}$$

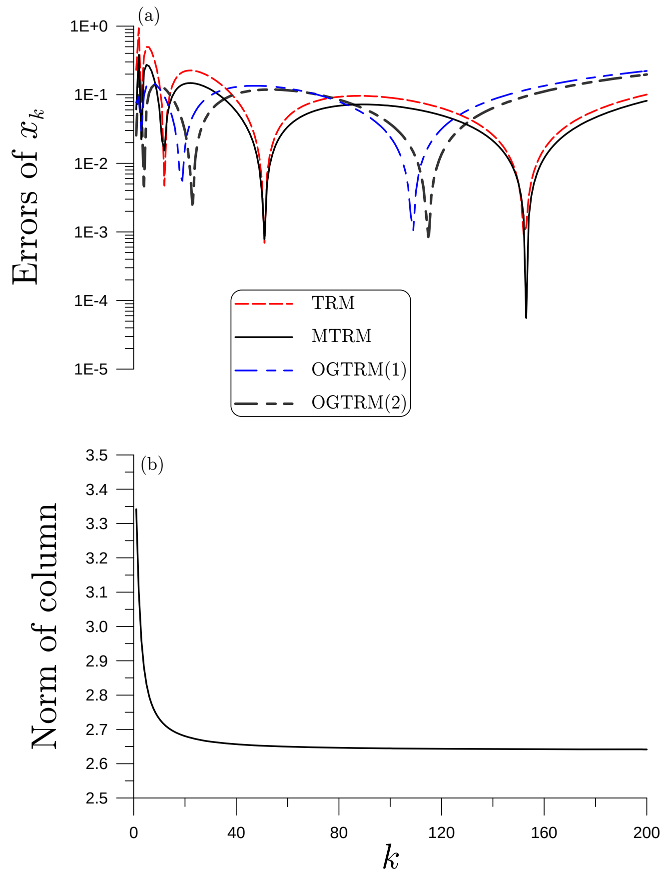

Figure 2: For example 2, (a) comparing the numerical errors obtained by the optimally generalized Tikhonov regularization methods [OGTRM(1), OGTRM(2)], the modified Tikhonov regularization method (MTRM), and Tikhonov regularization method (TRM), (b) the norm of column for the OGTRM(2).

we solve u under a final time condition:

$$u(x,T) = u^T(x). \tag{50}$$

The fundamental solution to Eq. (48) is given as follows:

$$K(x,t) = \frac{H(t)}{2\sqrt{\kappa\pi t}} \exp\left(\frac{-x^2}{4\kappa t}\right), \tag{51}$$

where $H(t)$ is the Heaviside function.

The method of fundamental solutions (MFS) has a broad application in engineering computations. However, the MFS has a serious drawback that the resulting linear equations system is always highly ill-conditioned, when the number of source points is increased [Golberg and Chen (1996)], or when the distances of source points are increased [Chen, Cho and Golberg (2006)].

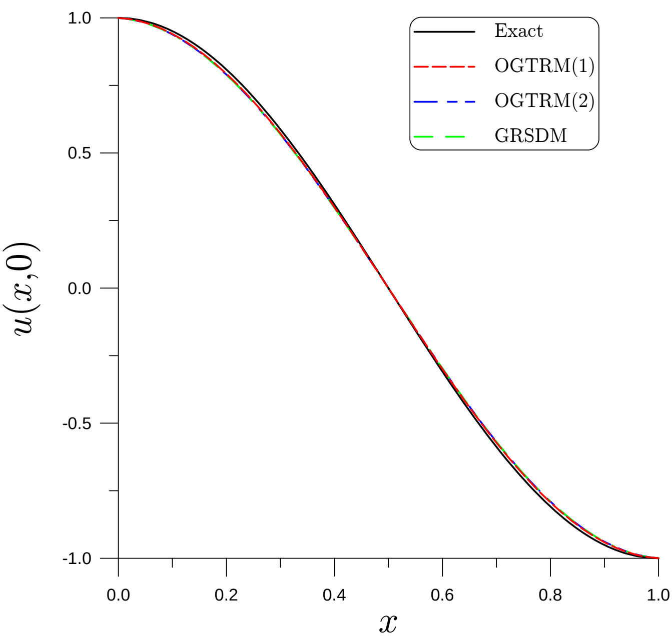

Figure 3: For example 3, comparing the numerical solutions obtained by the optimally generalized Tikhonov regularization methods [OGTRM(1), OGTRM(2)] and the GRSDM with the exact one.

In the MFS the solution of u at the field point $\mathbf{z} = (x,t)$ can be expressed as a linear combination of the fundamental solutions $U(\mathbf{z},\mathbf{s}_j)$:

$$u(\mathbf{z}) = \sum_{j=1}^{n} c_j U(\mathbf{z},\mathbf{s}_j), \ \ \mathbf{s}_j = (\eta_j, \tau_j) \in \Omega^c, \tag{52}$$

where n is the number of source points, c_j are unknown coefficients, and $\mathbf{s}_j$ are source points being located in the complement Ω^c of $\Omega = [0,\ell] \times [0,T]$. For the heat conduction equation we have the basis functions

$$U(\mathbf{z},\mathbf{s}_j) = K(x-\eta_j, t-\tau_j). \tag{53}$$

It is known that the location of source points in the MFS has a great influence on the accuracy and stability. In a practical application of MFS to solve the BHCP, the source points are uniformly located on two vertical straight lines parallel to the t-axis and one horizontal line over the final time, which was adopted by Hon and Li (2009) and Liu (2011b), showing a large improvement than the line location of source points below the initial time. After imposing the boundary conditions and the final time condition to Eq. (52) we can obtain a linear equations system:

$$\mathbf{V}\mathbf{x} = \mathbf{b}_1, \tag{54}$$

where

$$V_{ij} = U(\mathbf{z}_i, \mathbf{s}_j), \;\; \mathbf{x} = (c_1, \cdots, c_n)^{\mathrm{T}},$$
$$\mathbf{b}_1 = (u_\ell(t_i), \; i = 1, \ldots, m_1; u^T(x_j), \; j = 1, \ldots, m_2; u_0(t_k), \; k = m_1, \ldots, 1)^{\mathrm{T}}, \tag{55}$$

and $n = 2m_1 + m_2$.

Since the BHCP is highly ill-posed, the ill-condition of the coefficient matrix $\mathbf{V}$ in Eq. (54) is serious. To overcome the ill-posedness of Eq. (54) we can use the new methods to solve this problem. Here we compare the numerical solution with an exact solution:

$$u(x,t) = \cos(\pi x)\exp(-\pi^2 t).$$

For the case with $T = 1$ the value of final time data is in the order of 10^{-4}, which is small in a comparison with the value of the initial temperature $u_0(x) = \cos(\pi x)$ to be retrieved, which is $O(1)$. We solve this problem by the OGTRM(1) with $c_0 = 0$ and $\beta = 10^{-5}$, the OGTRM(2) with $c_0 = 1$ and $\beta = 10^{-8}$ and the GRSDM with $\mathbf{G} = \mathbf{I}_n$ and $\gamma = 0.1$. We have added a relative random noise with an intensity $\sigma = 10\%$ on the final time data, of which we compare the initial time data computed by the OGTRM(1), the OGTRM(2), and the GRSDM with the exact one in Fig. 3. The numerical errors are smaller than 0.0195 for the OGTRM(1) and OGTRM(2), and 0.0199 for the GRSDM. It indicates that the present iteratively regularized algorithms are robust against noise, and can provide quite accurate numerical results.

5.4 Inverse Cauchy problems

Let us consider the inverse Cauchy problem for the Laplace equation:

$$\Delta u = u_{rr} + \frac{1}{r}u_r + \frac{1}{r^2}u_{\theta\theta} = 0, \tag{56}$$

$$u(\rho, \theta) = h(\theta), \;\; 0 \le \theta \le \beta_0 \pi, \tag{57}$$

$$u_n(\rho, \theta) = g(\theta), \;\; 0 \le \theta \le \beta_0 \pi, \tag{58}$$

where $h(\theta)$ and $g(\theta)$ are given functions and $\beta_0 \leq 1$. The inverse Cauchy problem is given as follows:
To seek an unknown boundary function $f(\theta)$ on the part $\Gamma_2 := \{(r,\theta)|r = \rho(\theta),\ \beta_0\pi < \theta < 2\pi\}$ of the boundary under Eqs. (56)-(58) with the overspecified data on $\Gamma_1 := \{(r,\theta)|r = \rho(\theta),\ 0 \leq \theta \leq \beta_0\pi\}$.
It is well known that the method of fundamental solutions (MFS) can be used to solve the Laplace equation when a fundamental solution is known [Kupradze and Aleksidze (1964)]. In the MFS the solution of u at the field point $\mathbf{z} = (r\cos\theta, r\sin\theta)$ can be expressed as a linear combination of fundamental solutions $U(\mathbf{z},\mathbf{s}_j)$:

$$u(\mathbf{z}) = \sum_{j=1}^{n} c_j U(\mathbf{z},\mathbf{s}_j),\ \ \mathbf{s}_j \in \Omega^c. \tag{59}$$

For the Laplace equation (56) we have the fundamental solutions:

$$U(\mathbf{z},\mathbf{s}_j) = \ln r_j,\ \ r_j = \|\mathbf{z} - \mathbf{s}_j\|. \tag{60}$$

Previously, Liu (2008a) has proposed a new preconditioner to reduce the ill-condition of the MFS. In the practical application of MFS, by imposing the boundary conditions (57) and (58) to Eq. (59) we can obtain a linear equations system:

$$\mathbf{V}\mathbf{x} = \mathbf{b}_1, \tag{61}$$

where

$$\begin{aligned}
&\mathbf{z}_i = (z_i^1, z_i^2) = (\rho(\theta_i)\cos\theta_i, \rho(\theta_i)\sin\theta_i),\\
&\mathbf{s}_j = (s_j^1, s_j^2) = (R(\theta_j)\cos\theta_j, R(\theta_j)\sin\theta_j),\\
&V_{ij} = \ln\|\mathbf{z}_i - \mathbf{s}_j\|,\ \ \text{if } i \text{ is odd},\\
&V_{ij} = \frac{\eta(\theta_i)}{\|\mathbf{z}_i - \mathbf{s}_j\|^2}\left(\rho(\theta_i) - s_j^1\cos\theta_i - s_j^2\sin\theta_i - \frac{\rho'(\theta_i)}{\rho(\theta_i)}[s_j^1\sin\theta_i - s_j^2\cos\theta_i]\right),\\
&\qquad\qquad \text{if } i \text{ is even},
\end{aligned} \tag{62}$$

$$\mathbf{x} = (c_1,\ldots,c_n)^{\mathrm{T}},\ \ \mathbf{b}_1 = (h(\theta_1), g(\theta_1),\ldots,h(\theta_m), g(\theta_m))^{\mathrm{T}}, \tag{63}$$

in which $n = 2m$, and

$$\eta(\theta) = \frac{\rho(\theta)}{\sqrt{\rho^2(\theta) + [\rho'(\theta)]^2}}. \tag{64}$$

The above $R(\theta) = R$ with a constant R, or $R(\theta) = \rho(\theta) + D$ with a constant offset D can be used to locate the source points along a contour with a radius $R(\theta)$.

5.4.1 Example 4

For the purpose of comparison we consider the following exact solution:

$$u(r,\theta) = r^2 \cos(2\theta), \tag{65}$$

defined in a domain with the boundary $\rho(\theta) = \sqrt{10 - 6\cos(2\theta)}$, $0 \le \theta < 2\pi$.

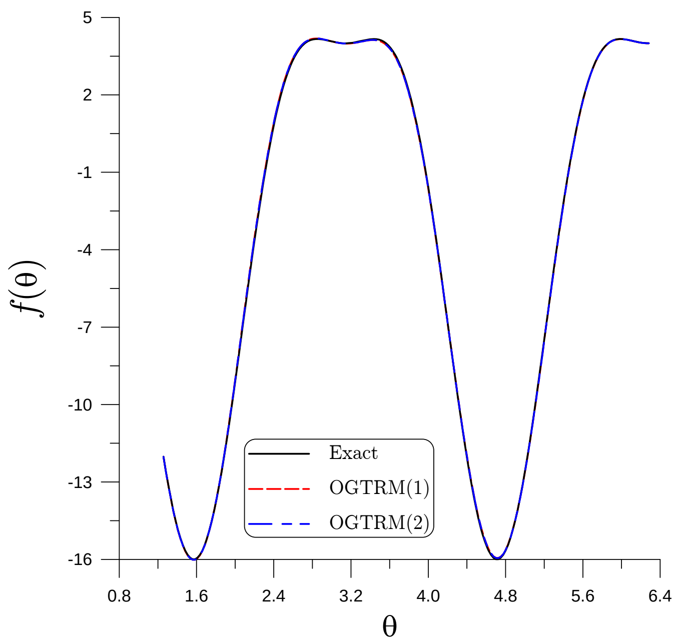

Figure 4: For example 4 comparing the numerical solutions obtained by OGTRM(1) and OGTRM(2) with the exact one.

We add a random noise with an intensity $\sigma = 1\%$ on the boundary data, and the numerical solutions on the boundary $\beta_0\pi < \theta < 2\pi$ with $\beta_0 = 0.4$ are computed by the OGTRM(1) with $\beta = 10^{-9}$ and $c_0 = 0$, and the OGTRM(2) with $\beta = 10^{-12}$ and $c_0 = 0$. For both methods we take $R = 15$ and $n = 40$ used in the MFS, and the convergence criteria are fixed to be $\varepsilon_1 = 10^{-5}$ and $\varepsilon_2 = 10^{-3}$. We compare the numerical solutions with the exact one in Fig. 4, where the maximum errors are both near to 0.1. When the OGTRM(1) is convergent with 48 iterations, the OGTRM(2) is convergent with only 24 iterations and with the maximum error being 0.09993. It indicates that the present algorithms of OGTRM(1) and OGTRM(2) are robust against noise, and the required data are parsimonious with $\beta_0 = 0.4$ only. To the best knowledge of the author, in the open literature there exist no other numerical

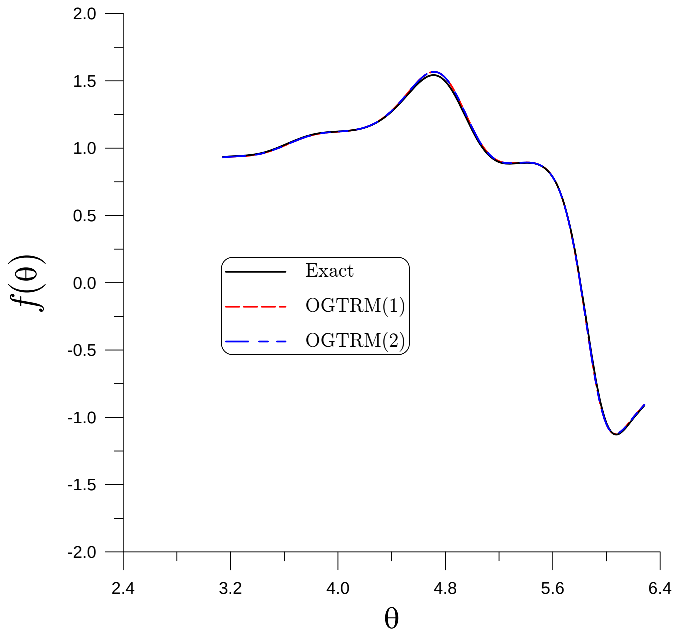

Figure 5: For example 5 comparing the numerical solutions obtained by OGTRM(1) and OGTRM(2) with the exact one.

methods can treat this type Cauchy problem with $\beta_0 = 0.4$. Previously, Liu (2008b) used the modified Trefftz method can treat a Cauchy problem with $\beta_0 = 0.5$.

5.4.2 Example 5

In the second example of the inverse Cauchy problem a complex amoeba-like irregular shape is adopted:

$$\rho(\theta) = \exp(\sin\theta)\sin^2(2\theta) + \exp(\cos\theta)\cos^2(2\theta). \tag{66}$$

We consider the following exact solution:

$$u(x,y) = \cos x \cosh y + \sin x \sinh y, \tag{67}$$

from which the exact boundary data can be derived. Here we fix $\beta_0 = 1$.

Under a random noise with an intensity $\sigma = 1\%$ being imposed on the boundary data, we compare the numerical solutions obtained by OGTRM(1) with $\beta = 10^{-10}$ and $c_0 = 0$, and OGTRM(2) with $\beta = 10^{-10}$ and $c_0 = 0$, with the exact one in

Fig. 5, where we take $D = 3$ and $n = 40$ for the use in the MFS. The maximum errors are both near to 0.027. When the OGTRM(1) is convergent with 179 iterations, the OGTRM(2) is convergent with 138 iterations. It indicates that the present algorithms of OGTRM(1) and OGTRM(2) are robust against noise.

6 Conclusions

In the present paper, we have introduced *four generalized and optimal regularization methods*. The new methods computed the approximate solution of ill-posed linear inverse problem by using the optimally-scaled preconditioning matrices. Different from the Tikhonov regularization method which drops out the regularized term on the right-hand side, the present iterative regularization methods do not drop out the regularized term on the right-hand side, do not perturb the original ill-posed linear equations system, and use the preconditioners and the inner iterations as the regularization tool to iteratively solve the ill-posed linear equations system. *In doing so we can retain both the regularization effect and the accuracy of numerical solutions*. We have proved that the iterative regularized solution sequences are monotonically convergent to the true solution. Several examples of ill-posed linear inverse problems were examined, which revealed that the MTRM, GRSDM, OGTRM(1) and OGTRM(2) have better computational efficiencies and accuracies than the classical Tikhonov-like regularization method.

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Appendix

In this appendix we derive the algorithm in Section 4. By Eq. (1):

$$\mathbf{F}(\mathbf{x}) = \mathbf{b}_1 - \mathbf{V}\mathbf{x}, \tag{A1}$$

we start from a continuous manifold:

$$h(\mathbf{x},t) := \frac{1}{2}Q(t)\|\mathbf{F}(\mathbf{x})\|^2 = C, \tag{A2}$$

where C is a positive constant. For the requirement of "consistency condition", i.e., $\mathbf{x}(t)$ is always on the manifold in time, we have

$$\frac{1}{2}\dot{Q}(t)\|\mathbf{F}(\mathbf{x})\|^2 - Q(t)\mathbf{r}\cdot\dot{\mathbf{x}} = 0, \tag{A3}$$

where $\mathbf{r} := \mathbf{V}^{\mathrm{T}}\mathbf{F}$. We suppose that $\mathbf{x}$ is governed by

$$\dot{\mathbf{x}} = \lambda \mathbf{G}\frac{\partial h}{\partial \mathbf{x}} = \lambda Q(t)\mathbf{G}\mathbf{r}, \tag{A4}$$

where λ is to be determined, and $\mathbf{G}$ is a positive definite matrix. Inserting Eq. (A4) into Eq. (A3) we can solve

$$\lambda = \frac{\dot{Q}(t)\|\mathbf{F}\|^2}{2Q^2(t)\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{r}}. \tag{A5}$$

Thus by inserting the above λ into Eq. (A4) we can obtain a nonlinear ODEs system for $\mathbf{x}$:

$$\dot{\mathbf{x}} = q(t)\frac{\|\mathbf{F}\|^2}{\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{r}}\mathbf{G}\mathbf{r}, \tag{A6}$$

where

$$q(t) := \frac{\dot{Q}(t)}{2Q(t)}. \tag{A7}$$

In order to keep $\mathbf{x}$ on the manifold we can consider the evolution of $\mathbf{F}$ along the path $\mathbf{x}(t)$ by

$$\dot{\mathbf{F}} = -\mathbf{V}\dot{\mathbf{x}} = -q(t)\frac{\|\mathbf{F}\|^2}{\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{r}}\mathbf{V}\mathbf{G}\mathbf{r}. \tag{A8}$$

Then, by Eq. (A2) we can derive

$$a(\Delta t)^2 - b\Delta t + 1 - \frac{Q(t)}{Q(t+\Delta t)} = 0, \tag{A9}$$

where

$$a := q^2(t)\frac{\|\mathbf{F}\|^2\mathbf{r}^{\mathrm{T}}\mathbf{GCGr}}{(\mathbf{r}^{\mathrm{T}}\mathbf{Gr})^2}, \tag{A10}$$

$$b := 2q(t). \tag{A11}$$

Inserting Eqs. (A10) and (A11) into Eq. (A9) we can derive

$$a_0(q\Delta t)^2 - 2(q\Delta t) + 1 - s = 0, \tag{A12}$$

where

$$s = \frac{Q(t)}{Q(t+\Delta t)}, \tag{A13}$$

$$a_0 := \frac{\|\mathbf{F}\|^2\mathbf{r}^{\mathrm{T}}\mathbf{GCGr}}{(\mathbf{r}^{\mathrm{T}}\mathbf{Gr})^2}. \tag{A14}$$

From Eq. (A12), we can take the solution of $q\Delta t$ to be

$$q\Delta t = \frac{1-\gamma}{a_0}, \tag{A15}$$

where $0 \le \gamma < 1$ is a relaxed parameter. After that, by applying the Euler method to integrate Eq. (A6) and using the above equation we can obtain the following algorithm:

$$\mathbf{x}(t+\Delta t) = \mathbf{x}(t) + (1-\gamma)\frac{\mathbf{r}^{\mathrm{T}}\mathbf{Gr}}{\mathbf{r}^{\mathrm{T}}\mathbf{GCGr}}\mathbf{Gr}. \tag{A16}$$

The reader can refer [Liu (2011a, 2012a); Liu and Atluri (2011a, 2011b, 2011c); Liu and Kuo (2011); Liu, Dai and Atluri (2011a, 2011b); Liu, Yeih, Kuo and Atluri (2009)] for other algorithms based on the concept of invariant manifold.