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An Optimal Preconditioner with an Alternate Relaxation Parameter Used to Solve Ill-Posed Linear Problems

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Abstract: In order to solve an ill-posed linear problem, we propose an innovative Jacobian type iterative method by presetting a conditioner before the steepest descent direction. The preconditioner is derived from an invariant manifold approach, which includes two parameters α and γ to be determined. When the weighting parameter α is optimized by minimizing a properly defined objective function, the relaxation parameter γ can be derived to accelerate the convergence speed under a switching criterion. When the switch is turned-on, by using the derived value of γ *it can pull back the iterative orbit to the* **fast manifold**. It is the first time that we have a formula for the relaxation parameter, by recognizing that γ is specified case by case, previously. The presently developed optimal and generalized steepest descent method with an alternate value of the relaxation parameter is able to overcome the ill-posedness of linear inverse problem, and provides a rather accurate numerical solution.

Keywords: Linear inverse problem, Ill-posed linear problem, Generalized relaxed steepest descent method (GRSDM), Optimal GRSDM (OGRSDM), Relaxation parameter, Optimal GRSDM with an Alternate Relaxation Parameter (OGRSDM-γ), Fast manifold

1 Introduction

In this paper we propose two innovative 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 a stable solution of such an ill-posed linear system has many

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important applications to linear inverse problems. In a practical situation of linear inverse problems which arise in engineering and scientific fields, 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 linear problem may deviate from the exact one to a great extent, when $\mathbf{V}$ is severely ill-conditioned and $\mathbf{b}_1$ is perturbed by random noise.

The approaches to solve the ill-posed linear problems can be categorized into three main classes: (a) regularizations of Eq. (1), (b) regularized algorithms to solve Eq. (1), and (c) a better preconditioning and/or postconditioning to Eq. (1). The matrix preconditioning technique is based on an approximation of the inverse of the coefficient matrix. In the splitting method we assume that $\mathbf{V} = \mathbf{M} - \mathbf{N}$ and associate it with an iterative method:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{M}^{-1}(\mathbf{b}_1 - \mathbf{V}\mathbf{x}_k). \tag{2}$$

Here $\mathbf{M}^{-1}$ plays the role of a preconditioner. The more $\mathbf{M}$ resembles $\mathbf{V}$, the faster the iterative method will converge. One of the natural and simplest ways for the choice of the preconditioner is a diagonal of the coefficient matrix, like as the Jacobi method. However, it usually has no remarkable reduction of the iteration number. To improve the convergence speed of iterative methods, an appropriate preconditioner can be incorporated. Based on the survey by Benzi (2002), a good preconditioner should meet the following requirements: (1) the preconditioned system should be easy to solve, and (2) the preconditioner should be cheap to construct and apply. In this paper we will propose a simple Jacobi type iterative method with its preconditioner being able to meet the above two requirements.

In the last few years, 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 (2012)], the best vector iterative method [Liu (2012d)], a globally optimal iterative method [Liu (2012e)], the generalized Tikhonov regularization methods [Liu (2012f)], as well as an optimal tri-vector iterative methods [Liu (2012g)].

The remainder of this paper is organized as follows. In Section 2, we first use a preset conditioner for solving an ill-posed linear system by a generalized relaxed steepest descent method (GRSDM). In Section 3 we search for an optimality of the preconditioner, where the preconditioned matrix is optimized based on the concepts of invariant manifold and the maximization of convergence rate derived from a properly defined objective function. In Section 4 we derive a formula to compute the relaxation parameter introduced in the preconditioner; hence, we can design a new strategy by enlarging the stepsize when a situation for a faster convergence is detected. In Section 5 we give numerical examples of backward heat conduction problem, heat source identification problem, and inverse Cauchy problems to demonstrate the efficiency and accuracy of the novel iterative algorithms. Finally, the conclusions are drawn in Section 6.

2 A generalized relaxed steepest descent method

Considering the following preconditioner:

$$\mathbf{P} := \mathbf{V}^{\mathrm{T}} - \mathbf{E}^{-1}\mathbf{V}^{-1}, \tag{3}$$

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

$$(\mathbf{V}^{\mathrm{T}}\mathbf{V} - \mathbf{E}^{-1})\mathbf{x} = \mathbf{b} - \mathbf{E}^{-1}\mathbf{x}, \tag{4}$$

where $\mathbf{E}$ is a positive definite matrix. The term $\mathbf{E}^{-1}\mathbf{x}$ in the right-hand side is obtained from $\mathbf{E}^{-1}\mathbf{V}^{-1}\mathbf{b}_1 = \mathbf{E}^{-1}\mathbf{x}$ by using Eq. (1) again.
Hence, we have an iterative scheme to find the solution of $\mathbf{x}$ by

$$(\mathbf{V}^{\mathrm{T}}\mathbf{V} - \mathbf{E}^{-1})\mathbf{x}_k = \mathbf{b} - \mathbf{E}^{-1}\mathbf{x}_{k+1}, \tag{5}$$

which is obtained from Eq. (4) by letting $\mathbf{x} = \mathbf{x}_k$ in the left-hand side, and simultaneously letting $\mathbf{x} = \mathbf{x}_{k+1}$ in the right-hand side. Thus we can derive

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{E}\mathbf{r}_k, \tag{6}$$

where

$$\mathbf{r}_k = \mathbf{b} - \mathbf{C}\mathbf{x}_k \tag{7}$$

is a residual vector (usually named the steepest descent direction) for the normal equation:

$$\mathbf{C}\mathbf{x} = \mathbf{b}, \tag{8}$$

in which

$$\mathbf{C} := \mathbf{V}^{\mathrm{T}}\mathbf{V}, \tag{9}$$

$$\mathbf{b} := \mathbf{V}^{\mathrm{T}}\mathbf{b}_1. \tag{10}$$

In the next section we will search $\mathbf{E}$ as an optimal preconditioner, such that the iterative algorithm (6) can converge faster through the left-action of the preconditioned matrix $\mathbf{E}$ on $\mathbf{r}_k$. Hereby, upon taking

$$\mathbf{E} = (1-\gamma)\frac{\mathbf{r}_k^{\mathrm{T}}\mathbf{G}\mathbf{r}_k}{\mathbf{r}_k^{\mathrm{T}}\mathbf{G}\mathbf{C}\mathbf{G}\mathbf{r}_k}\mathbf{G} \tag{11}$$

in Eq. (6), we can derive the following algorithm:
(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:

$$\mathbf{r}_k = \mathbf{b} - \mathbf{C}\mathbf{x}_k, \tag{12}$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + (1-\gamma)\frac{\mathbf{r}_k^{\mathrm{T}}\mathbf{G}\mathbf{r}_k}{\mathbf{r}_k^{\mathrm{T}}\mathbf{G}\mathbf{C}\mathbf{G}\mathbf{r}_k}\mathbf{G}\mathbf{r}_k. \tag{13}$$

If $\mathbf{x}_{k+1}$ converges by satisfying a given stopping criterion $\|\mathbf{r}_{k+1}\| < \varepsilon$, then stop; otherwise, go to step (ii).

In Eq. (13), γ is a relaxation parameter in the range of $0 \leq \gamma < 1$, and if we take $\mathbf{G} = \mathbf{I}_n$, then the above algorithm reduces to the relaxed steepest descent method (RSDM) developed by Liu (2011a, 2012a). If we take $\mathbf{G} = \mathbf{V}^{\mathrm{T}}\mathbf{V}$, $\mathbf{G} = \mathbf{V}\mathbf{V}^{\mathrm{T}}$, or else, we can obtain different algorithms. Consequently, the present algorithm can be viewed as a generalized relaxed steepest descent method (GRSDM), with $\mathbf{G}$ being positive-definite. In the next section we will search an optimal $\mathbf{G} = \mathbf{I}_n + \alpha\mathbf{D}$ with the weighting parameter α being optimized, where $\mathbf{D}$ is a positive definite matrix specified by the user. When $\alpha = 0$, we recover to the RSDM. In Eq. (13), we can view the preset matrix $(1-\gamma)\mathbf{r}_k^{\mathrm{T}}\mathbf{G}\mathbf{r}_k/(\mathbf{r}_k^{\mathrm{T}}\mathbf{G}\mathbf{C}\mathbf{G}\mathbf{r}_k)\mathbf{G}$ before the steepest descent direction $\mathbf{r}_k$ as being a preconditioner. In our previous studies, the relaxation parameter γ was specified case by case. Its value is dependent on the problem we solve, and is chosen by the user. In Section 4, we will derive a *formula to compute the relaxation parameter γ under a switching criterion*, such that γ is either using the specified value or using a value computed from the derived formula. In our experience, the value of γ has a prominent influence on the convergence speed.

3 An invariant manifold approach

In this section we revise the iterative algorithm in Section 2, and search an optimization of the preconditioner $\mathbf{G}$. By Eq. (1):

$$\mathbf{F}(\mathbf{x}) = \mathbf{b}_1 - \mathbf{V}\mathbf{x}, \tag{14}$$

we start from a continuous manifold:

$$h(\mathbf{x},t) := \frac{1}{2}Q(t)\|\mathbf{F}(\mathbf{x})\|^2 = C, \tag{15}$$

where C is a positive constant, and the function $Q(t) \in \mathbb{C}^1$ satisfies $Q(0) = 1$ and $\dot{Q}(t) > 0$. For the requirement of "consistency condition", i.e., $\mathbf{x}(t)$ is always on the manifold in time, we have

$$\frac{1}{2}\dot{Q}(t)\|\mathbf{F}(\mathbf{x})\|^2 - Q(t)\mathbf{r}\cdot\dot{\mathbf{x}} = 0, \tag{16}$$

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

$$\dot{\mathbf{x}} = \lambda\mathbf{G}\frac{\partial h}{\partial \mathbf{x}} = \lambda Q(t)\mathbf{G}\mathbf{r}, \tag{17}$$

where λ is to be determined, and $\mathbf{G}$ is a positive definite matrix. Inserting Eq. (17) into Eq. (16) we can solve

$$\lambda = \frac{\dot{Q}(t)\|\mathbf{F}\|^2}{2Q^2(t)\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{r}}. \tag{18}$$

Thus by inserting the above λ into Eq. (17) we have a nonlinear ODEs system for $\mathbf{x}$:

$$\dot{\mathbf{x}} = q(t)\frac{\|\mathbf{F}\|^2}{\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{r}}\mathbf{G}\mathbf{r}, \tag{19}$$

where

$$q(t) := \frac{\dot{Q}(t)}{2Q(t)}. \tag{20}$$

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

$$\dot{\mathbf{F}} = -\mathbf{V}\dot{\mathbf{x}} = -q(t)\frac{\|\mathbf{F}\|^2}{\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{r}}\mathbf{V}\mathbf{G}\mathbf{r}, \tag{21}$$

and by applying the Euler method we have

$$\mathbf{F}(t+\Delta t) = \mathbf{F}(t) - q(t)\Delta t \frac{\|\mathbf{F}(t)\|^2}{\mathbf{r}^{\mathrm{T}}(t)\mathbf{G}\mathbf{r}(t)} \mathbf{V}\mathbf{G}\mathbf{r}(t). \tag{22}$$

Then, by Eq. (15) we can derive

$$a(\Delta t)^2 - b\Delta t + 1 - \frac{Q(t)}{Q(t+\Delta t)} = 0, \tag{23}$$

where

$$a := q^2(t) \frac{\|\mathbf{F}\|^2 \mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{C}\mathbf{G}\mathbf{r}}{(\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{r})^2}, \tag{24}$$

$$b := 2q(t). \tag{25}$$

Inserting Eqs. (24) and (25) into Eq. (23) we can derive a scalar equation to solve the stepsize η:

$$a_0\eta^2 - 2\eta + 1 - s = 0, \tag{26}$$

where

$$\eta := q(t)\Delta t, \tag{27}$$

$$s := \frac{Q(t)}{Q(t+\Delta t)} = \frac{\|\mathbf{F}(t+\Delta t)\|^2}{\|\mathbf{F}(t)\|^2}, \tag{28}$$

$$a_0 := \frac{\|\mathbf{F}\|^2 \mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{C}\mathbf{G}\mathbf{r}}{(\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{r})^2}. \tag{29}$$

By using Eq. (9) and $\mathbf{r} = \mathbf{V}^{\mathrm{T}}\mathbf{F}$, a_0 can be written as

$$a_0 = \frac{\|\mathbf{F}\|^2 \|\mathbf{V}\mathbf{G}\mathbf{V}^{\mathrm{T}}\mathbf{F}\|^2}{[\mathbf{F}\cdot(\mathbf{V}\mathbf{G}\mathbf{V}^{\mathrm{T}}\mathbf{F})]^2} \geq 1, \tag{30}$$

of which the inequality follows from the Cauchy-Schwarz inequality.

From Eq. (26) we have a preferred solution of η to be

$$\eta = \frac{1-\sqrt{1-(1-s)a_0}}{a_0}, \ \text{ if } 1-(1-s)a_0 \geq 0. \tag{31}$$

Let

$$1-(1-s)a_0 = \gamma^2 \geq 0; \tag{32}$$

such that the condition $1-(1-s)a_0 \geq 0$ in Eq. (31) is automatically satisfied. From Eqs. (32) and (31) it follows that

$$s = 1 - \frac{1-\gamma^2}{a_0}, \tag{33}$$

$$\eta = \frac{1-\gamma}{a_0}, \tag{34}$$

where γ satisfying

$$0 \leq \gamma < 1 \tag{35}$$

is a relaxation parameter.

Then, by applying the Euler method to integrate Eq. (19) and using Eq. (34) for $\eta = q(t)\Delta t$ we can obtain

$$\mathbf{x}(t+\Delta t) = \mathbf{x}(t) + (1-\gamma)\frac{\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{r}}{\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{C}\mathbf{G}\mathbf{r}}\mathbf{G}\mathbf{r}, \tag{36}$$

which was already shown in Eq. (13) as an iterative algorithm.

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 iterative algorithms based on the concept of invariant manifold.

Under conditions (30) and (35), from Eqs. (28) and (33) it follows that

$$\frac{\|\mathbf{F}(t+\Delta t)\|}{\|\mathbf{F}(t)\|} = \sqrt{s} < 1, \tag{37}$$

which means that the residual error is absolutely decreased. In other words, the convergence rate of present iterative algorithm satisfies

$$\text{Convergence Rate (CR)} := \frac{\|\mathbf{F}(t)\|}{\|\mathbf{F}(t+\Delta t)\|} = \frac{1}{\sqrt{s}} > 1. \tag{38}$$

The property in Eq. (38) is very important, since it guarantees that the new algorithm is absolutely convergent to the true solution. *A smaller s will lead to a faster convergence.*

Now, we let

$$\mathbf{G} = \mathbf{I}_n + \alpha\mathbf{D}, \tag{39}$$

where α is a weighting parameter to be optimized, and $\mathbf{D}$ is a positive definite matrix. From Eq. (39) it follows that

$$(\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{r})^2 = (\|\mathbf{r}\|^2 + \alpha\|\mathbf{r}\|_D^2)^2, \tag{40}$$

where

$$\|\mathbf{r}\|_D^2 := \mathbf{r}^{\mathrm{T}}\mathbf{D}\mathbf{r} \tag{41}$$

is the squared D-norm of $\mathbf{r}$, and also that

$$\mathbf{r}^{\mathrm{T}}\mathbf{G}\mathbf{C}\mathbf{G}\mathbf{r} = \|\mathbf{V}\mathbf{G}\mathbf{r}\|^2 = \|\mathbf{v}_1 + \alpha\mathbf{v}_2\|^2, \tag{42}$$

where

$$\mathbf{v}_1 := \mathbf{V}\mathbf{r}, \;\; \mathbf{v}_2 := \mathbf{V}\mathbf{D}\mathbf{r}. \tag{43}$$

Inserting Eqs. (40) and (42) into Eq. (29) we can derive

$$a_0 = \frac{\|\mathbf{F}\|^2(\|\mathbf{v}_1\|^2 + 2\alpha\mathbf{v}_1\cdot\mathbf{v}_2 + \alpha^2\|\mathbf{v}_2\|^2)}{(\|\mathbf{r}\|^2 + \alpha\|\mathbf{r}\|_D^2)^2}. \tag{44}$$

Thus by Eqs. (38) and (33) we can choose the optimal value of α by letting $\partial s/\partial\alpha = 0$, i.e., $\partial a_0/\partial\alpha = 0$. Through some elementary operations on Eq. (44) we can derive

$$\alpha = \frac{\|\mathbf{r}\|^2\mathbf{v}_1\cdot\mathbf{v}_2 - \|\mathbf{r}\|_D^2\|\mathbf{v}_1\|^2}{\|\mathbf{r}\|_D^2\mathbf{v}_1\cdot\mathbf{v}_2 - \|\mathbf{r}\|^2\|\mathbf{v}_2\|^2}. \tag{45}$$

Under the above weighting parameter of α in the preconditioned matrix $\mathbf{G} = \mathbf{I}_n + \alpha\mathbf{D}$, s can be minimized; hence, the convergence rate $1/\sqrt{s}$ will be maximized.

4 An alternate value of relaxation parameter

In the above the relaxation parameter γ is not yet specified. Here we can derive a formula about γ.

By using the Euler method we have

$$\dot{Q}(t)\Delta t = Q(t+\Delta t) - Q(t). \tag{46}$$

From Eqs. (27), (20), (28) and (46) we have

$$\eta = q(t)\Delta t = \frac{\dot{Q}(t)\Delta t}{2Q(t)} = \frac{1}{2s} - \frac{1}{2}. \tag{47}$$

Then by Eqs. (34) and (47) we can obtain

$$s = \frac{1}{2\eta+1} = \frac{a_0}{a_0 + 2 - 2\gamma}. \tag{48}$$

On the other hand, Eq. (33) renders

$$s = \frac{a_0 - 1 + \gamma^2}{a_0}. \tag{49}$$

By equating the two s in the above two equations, we can derive a third-order scalar equation for γ:

$$2\gamma^3 - (a_0 + 2)\gamma^2 + 2(a_0 - 1)\gamma - a_0 + 2 = 0. \tag{50}$$

Fortunately, we can decompose the above equation into

$$2(\gamma - 1)^2 \left(\gamma - \frac{a_0}{2} + 1\right) = 0, \tag{51}$$

where $\gamma = 1$ is a double roots, which is not the desired one in view of Eq. (35), and another is

$$\gamma = \frac{a_0}{2} - 1, \;\text{ if }\; 2 \le a_0 < 4, \tag{52}$$

where, in order to satisfy Eq. (35), we impose the condition of $2 \le a_0 < 4$.

Liu (2012h) has derived another form of s. From Eqs. (20), (27) and (46) it follows that

$$\eta = \frac{1}{2}(R - 1), \tag{53}$$

where the ratio R is defined by

$$R := \frac{Q(t + \Delta t)}{Q(t)} = \frac{1}{s}. \tag{54}$$

Inserting Eqs. (53) and (54) into Eq. (26) we can derive

$$a_0 R^3 - 2(a_0 + 2)R^2 + (a_0 + 8)R - 4 = 0. \tag{55}$$

It is interesting that the above equation can be written as

$$(R - 1)^2 (a_0 R - 4) = 0. \tag{56}$$

To satisfy the requirement of $\dot{Q}(t) > 0$, we need $R > 1$. Because $R = 1$ is a double roots and it is not the desired one, we can take

$$R = \frac{4}{a_0}. \tag{57}$$

Thus, besides Eqs. (48) and (49), by Eqs. (54) and (57) we have obtained the third representation of s:

$$s = \frac{a_0}{4}. \tag{58}$$

By equating Eqs. (58) and (48) we obtain the same solution for γ as that in Eq. (52). However, if we let the two s in Eqs. (58) and (49) be equal, we can solve

$$\gamma^2 = \left(\frac{a_0}{2} - 1\right)^2. \tag{59}$$

In summary, we can set

$$\gamma = \left|\frac{a_0}{2} - 1\right|, \text{ if } a_0 < 4, \tag{60}$$

where we restrict $a_0 < 4$ in order to satisfy Eq. (35).

Hence, we have developed an optimal GRSDM with an alternate value of γ (OGRSDM-γ):

(i) Select a suitable value of $0 \le \gamma_0 < 1$, a positive-definite matrix $\mathbf{D}$, and assume an initial value of $\mathbf{x}_0$.

(ii) For $k = 0, 1, 2 \dots$ we repeat the following computations:

$$\mathbf{F}_k = \mathbf{b}_1 - \mathbf{V}\mathbf{x}_k,$$
$$\mathbf{r}_k = \mathbf{b} - \mathbf{C}\mathbf{x}_k,$$
$$\|\mathbf{r}_k\|_D^2 = \mathbf{r}_k \cdot (\mathbf{D}\mathbf{r}_k),$$
$$\mathbf{v}_1^k = \mathbf{V}\mathbf{r}_k,$$
$$\mathbf{v}_2^k = \mathbf{V}\mathbf{D}\mathbf{r}_k,$$
$$\alpha_k = \frac{\|\mathbf{r}_k\|^2 \mathbf{v}_1^k \cdot \mathbf{v}_2^k - \|\mathbf{r}_k\|_D^2 \|\mathbf{v}_1^k\|^2}{\|\mathbf{r}_k\|_D^2 \mathbf{v}_1^k \cdot \mathbf{v}_2^k - \|\mathbf{r}_k\|^2 \|\mathbf{v}_2^k\|^2},$$
$$\mathbf{G}_k = \mathbf{I}_n + \alpha_k \mathbf{D},$$
$$a_0^k = \frac{\|\mathbf{F}_k\|^2 (\mathbf{G}_k\mathbf{r}_k) \cdot (\mathbf{C}\mathbf{G}_k\mathbf{r}_k)}{[\mathbf{r}_k \cdot (\mathbf{G}_k\mathbf{r}_k)]^2},$$
$$\gamma = \begin{cases} \left|\frac{a_0^k}{2} - 1\right|, & \text{if } a_0^k < 4, \\ \gamma_0, & \text{otherwise,} \end{cases} \tag{61}$$
$$\mathbf{x}_{k+1} = \mathbf{x}_k + (1-\gamma)\frac{\mathbf{r}_k \cdot (\mathbf{G}_k\mathbf{r}_k)}{(\mathbf{G}_k\mathbf{r}_k) \cdot (\mathbf{C}\mathbf{G}_k\mathbf{r}_k)}\mathbf{G}_k\mathbf{r}_k. \tag{62}$$

If $\mathbf{x}_{k+1}$ converges by satisfying a given stopping criterion $\|\mathbf{r}_{k+1}\| < \varepsilon$, then stop; otherwise, go to step (ii). If γ is fixed to be the selected value γ_0, then the resultant algorithm is an optimal GRSDM (OGRSDM).

Previously, the value of relaxation parameter γ is specified by the user case by case. Here we have derived a formula to compute γ by $\gamma = |a_0/2 - 1|$ under a switching criterion $a_0 < 4$ in Eq. (61), such that γ is either using the specified value γ_0 or using a value computed from $\gamma = |a_0/2 - 1|$, depending on the value of a_0. Numerical examples given below will explore the efficiency by designing a switching formula for the relaxation parameter γ.

Remark: Another choice of the switching criterion in Eq. (61) might be

$$2(1-\gamma_0) < a_0 < 2(1+\gamma_0). \tag{63}$$

In order to derive the above switching criterion, let us denote the value of s by s_0:

$$s_0 = 1 - \frac{1-\gamma_0^2}{a_0}, \tag{64}$$

when one inserts γ_0 into Eq. (33). Correspondingly, when we insert Eq. (60) for γ into Eq. (33) we can derive

$$s = \frac{a_0}{4} \tag{65}$$

as shown in Eq. (58). Thus for a smaller value of s than s_0 (i.e., for a faster convergence gained by using s) we can derive

$$\frac{a_0}{4} < 1 - \frac{1-\gamma_0^2}{a_0}, \tag{66}$$

which can be recast to

$$(a_0-2)^2 < 4\gamma_0^2. \tag{67}$$

Taking the square roots of both sides we can derive Eq. (63). However, the width of the range for a_0 in Eq. (63) is only $4\gamma_0$. When γ_0 is a small value, say $\gamma_0 = 0.05$, the width of the range is 0.2. In practice, the switching criterion in Eq. (63) maybe not have a chance to work because the probability that a_0 locates in such a small range is very small. So, in this study the OGRSDM-γ did not use the switching criterion in Eq. (63); instead of we use $a_0 < 4$ in Eq. (61).

5 Numerical examples

Below, we use some well-known ill-posed linear problems and linear inverse problems to validate the performance of OGRSDM and OGRSDM-γ in solving ill-posed linear problems.

5.1 Hilbert linear problem

Finding an n-order polynomial function $p(x) = a_0 + a_1 x + \ldots + a_n x^n$ to best match a continuous function $f(x)$ in the interval of $x \in [0,1]$:

$$\min_{\deg(p) \leq n} \int_0^1 [f(x) - p(x)]^2 dx, \tag{68}$$

leads to a problem governed by Eq. (1), where $\mathbf{V}$ is the $(n+1) \times (n+1)$ Hilbert matrix, defined by

$$V_{ij} = \frac{1}{i+j-1}, \tag{69}$$

$\mathbf{x}$ is composed of the $n+1$ coefficients $a_0, a_1, \ldots, a_n$ appeared in $p(x)$, and

$$\mathbf{b} = \begin{bmatrix} \int_0^1 f(x)dx \\ \int_0^1 x f(x)dx \\ \vdots \\ \int_0^1 x^n f(x)dx \end{bmatrix} \tag{70}$$

is uniquely determined by the function $f(x)$.

The Hilbert matrix is a famous example of highly ill-conditioned matrices. Eq. (1) with the coefficient matrix $\mathbf{V}$ having a large condition number usually displays that an arbitrarily small perturbation of data on the right-hand side may lead to an arbitrarily large perturbation to the solution on the left-hand side.

Let us consider a highly ill-posed case of this problem with $n = 50$. For this problem the condition number is about 1.1748×10^{19}. We consider a constant solution $x_1 = x_2 = \ldots = x_{50} = 1$. The noise σ is fixed to be 10^{-5}, while the convergence criterion is fixed to be $\varepsilon = 10^{-4}$. Starting from the initial conditions with $x_i = 0.5,\ i = 1, \ldots, 50$, the OGRSDM with $\gamma_0 = 0.9$ and with $\mathbf{D} = \mathbf{V}^{\mathrm{T}}\mathbf{V}$ converges with 15868 iterations, but the OGRSDM-γ with $\gamma_0 = 0.9$ and with $\mathbf{D} = \mathbf{V}^{\mathrm{T}}\mathbf{V}$ converges with 4861 iterations as shown in Fig. 1(a) for the residual errors. The values of γ for the OGRSDM-γ is shown in Fig. 1(b), and the values of a_0 for OGRSDM and OGRSDM-γ are compared in Fig. 1(c). We can appreciate that the switching criterion designed for the OGRSDM-γ can enhance the convergence speed. When the switch is turned-on, by using the derived value of $\gamma = |a_0/2 - 1|$ it can pull back the iterative orbit to the **fast manifold** as shown in Fig. 1(a) for the large reductions of residual error at these spikes of γ in Fig. 1(b). Both the numerical errors of OGRSDM and OGRSDM-γ are smaller than 0.024.

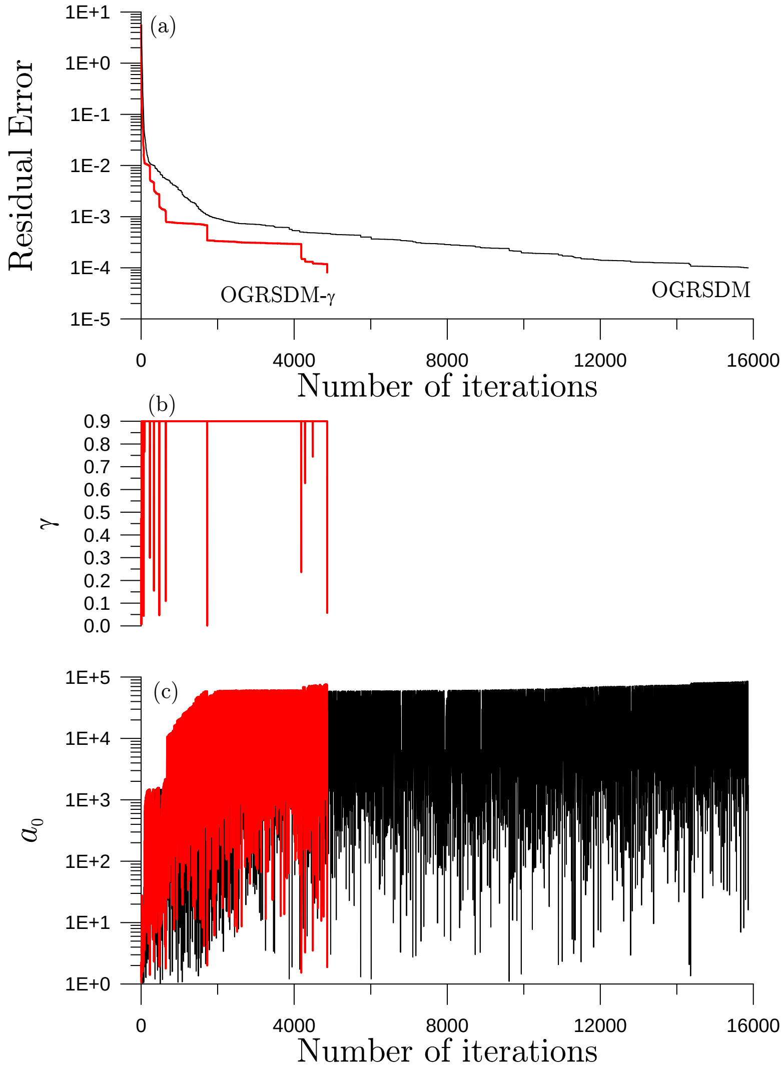

Figure 1: For a Hilbert linear problem with $n = 50$, (a) comparing the residual errors, (b) the value of γ for OGRSDM- γ, and (c) comparing a_0.

In order to investigate the influence of γ_0 on the number of iterations for OGRSDM and OGRSDM-γ, we plot them in Fig. 2(a) with respect to γ_0. It can be seen that the OGRSDM-γ is convergent faster than the OGRSDM when γ_0 is greater than 0.6. Moreover, as shown in Fig. 2(b) the maximum errors obtained by the OGRSDM-γ

are smaller than that obtained by the OGRSDM.

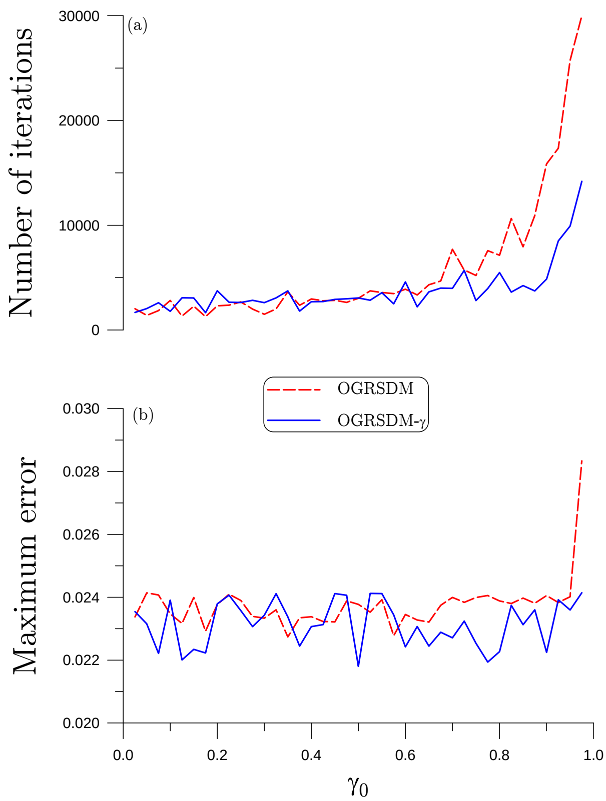

Figure 2: For a Hilbert linear problem, (a) comparing the number of iterations, and (b) the maximum errors of OGRSDM and OGRSDM-γ with respect to γ_0.

5.2 *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:

$$u_t(x,t) = \kappa u_{xx}(x,t), \;\; 0 < t < T, \;\; 0 < x < \ell, \tag{71}$$

$$u(0,t) = u_0(t), \;\; u(\ell,t) = u_\ell(t), \tag{72}$$

we solve u under a final time condition:

$$u(x,T) = u^T(x). \tag{73}$$

The fundamental solution of Eq. (71) is given as follows:

$$K(x,t) = \frac{H(t)}{2\sqrt{\kappa\pi t}} \exp\left(\frac{-x^2}{4\kappa t}\right), \tag{74}$$

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

The method of fundamental solutions (MFS) has a broad applications in engineering computation. 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)].

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 $U(\mathbf{z},\mathbf{s}_j)$:

$$u(\mathbf{z}) = \sum_{j=1}^{n} c_j U(\mathbf{z},\mathbf{s}_j), \;\; \mathbf{s}_j = (\eta_j, \tau_j) \in \Omega^c, \tag{75}$$

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

$$U(\mathbf{z},\mathbf{s}_j) = K(x-\eta_j, t-\tau_j). \tag{76}$$

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 not 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. (75) we can obtain a linear equations system:

$$\mathbf{V}\mathbf{x} = \mathbf{b}_1, \tag{77}$$

where

$$\begin{aligned} &V_{ij} = U(\mathbf{z}_i,\mathbf{s}_j), \;\; \mathbf{x} = (c_1,\cdots,c_n)^{\mathrm{T}}, \\ &\mathbf{b}_1 = (u_\ell(t_i),\ i=1,\ldots,m_1; u^T(x_j),\ j=1,\ldots,m_2; u_0(t_k),\ k=m_1,\ldots,1)^{\mathrm{T}}, \end{aligned} \tag{78}$$

and $n = 2m_1 + m_2$.

Example 1: Since the BHCP is highly ill-posed, the ill-condition of the coefficient matrix $\mathbf{V}$ in Eq. (77) is serious. To overcome the ill-posedness of Eq. (77) 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 much smaller than the value of the initial temperature $u_0(x) = \cos(\pi x)$ to be retrieved, which is $O(1)$. By adding a relative random noise with an intensity $\sigma = 10\%$ on the final time data, we compute the initial time data by the GRSDM [Liu (2012f)] with $\mathbf{G} = \mathbf{I}_n$, and the OGRSDM and the OGRSDM-γ with $\mathbf{D} = \mathbf{C} = \mathbf{V}^{\mathrm{T}}\mathbf{V}$.

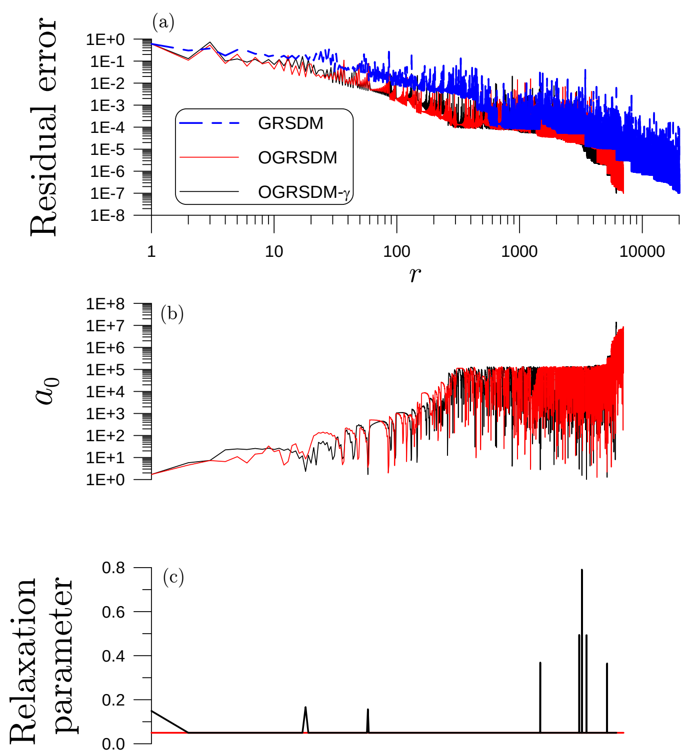

Figure 3: For example 1, (a) comparing the residual errors, (b) and (c) the value of a_0 and the relaxation parameters of OGRSDM (red) and OGRSDM-γ (black).

When the GRSDM with $\gamma = 0.05$ spends 20050 iterations to satisfy the convergence criterion $\varepsilon = 10^{-7}$, the OGRSDM spends 7025 iterations and the OGRSDM-γ is the fastest one with 6164 iterations. The residual errors of the above three methods

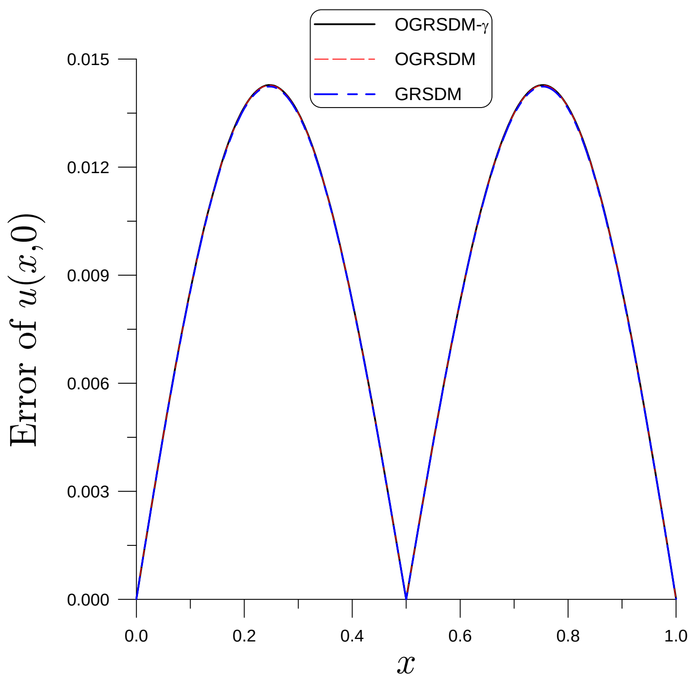

Figure 4: For example 1 comparing the numerical errors of GRSDM, OGRSDM and OGRSDM-γ.

are compared in Fig. 3(a). The values of a_0 and γ for the OGRSDM and OGRSDM-γ are compared, respectively, in Figs. 3(b) and 3(c). From Fig. 3(c) it can be seen that the OGRSDM-γ has eight times by using the larger values of γ, such that the OGRSDM-γ can converge faster than the OGRSDM, which used a constant value of $\gamma_0 = 0.05$, . For the above three methods the numerical errors as shown in Fig. 4 are all smaller than 0.015. This example indicates that the present iterative algorithms are robust against noise, and can provide quite accurate numerical results.

In order to investigate the influence of γ_0 on the number of iterations of OGRSDM and OGRSDM-γ, we plot them in Fig. 5 with respect to γ_0. It can be seen that the OGRSDM-γ is convergent faster than the OGRSDM when γ_0 is greater than 0.5.

5.3 Heat source identification problem

In this section we apply the OGRSDM and OGRSDM-γ to identify an unknown space-dependent heat source function $H(x)$ for a one-dimensional heat conduction

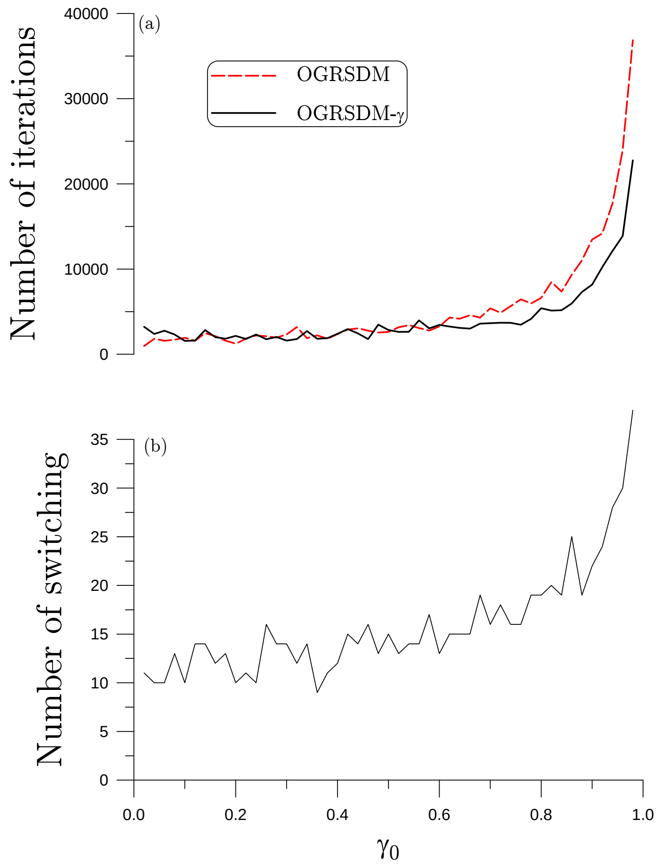

Figure 5: For example 1, (a) comparing the number of iterations of OGRSDM and OGRSDM-γ, and (b) showing the number of switching for OGRSDM-γ.

equation:

$$u_t(x,t) = u_{xx}(x,t) + H(x),\ 0 < x < \ell,\ 0 < t < t_f, \tag{79}$$

$$u(0,t) = u_0(t),\ \ u(\ell,t) = u_\ell(t), \tag{80}$$

$$u(x,0) = f(x). \tag{81}$$

In order to identify $H(x)$ we can impose an extra condition:

$$u_x(0,t) = q(t). \tag{82}$$

We propose a numerical differential method by letting $v = u_t$. Taking the differentials of Eqs. (79) and (80) and (82) with respect to t, and letting $v = u_t$ we can derive

$$v_t(x,t) = v_{xx}(x,t),\ 0 < x < \ell,\ 0 < t < t_f, \tag{83}$$
$$v(0,t) = \dot{u}_0(t), \tag{84}$$
$$v(\ell,t) = \dot{u}_\ell(t), \tag{85}$$
$$v_x(0,t) = \dot{q}(t). \tag{86}$$

This is an inverse heat conduction problem (IHCP) for $v(x,t)$ without using the initial condition.

Therefore as being a numerical method, we can first solve the above IHCP for $v(x,t)$ by using the MFS in Section 5.2 to obtain a linear equations system and then the method introduced in Section 4 is used to solve the resultant linear equations system; hence, we can construct $u(x,t)$ by

$$u(x,t) = \int_0^t v(x,\xi)d\xi + f(x), \tag{87}$$

which automatically satisfies the initial condition in Eq. (81).

From Eq. (87) it follows that

$$u_{xx}(x,t) = \int_0^t v_{xx}(x,\xi)d\xi + f''(x), \tag{88}$$

which together with $u_t = v$ as being inserted into Eq. (79), leads to

$$v(x,t) = \int_0^t v_{xx}(x,\xi)d\xi + f''(x) + H(x). \tag{89}$$

Inserting Eq. (83) for $v_{xx} = v_t$ into the above equation and integrating it we can derive the following equation to recover $H(x)$:

$$H(x) = v(x,0) - f''(x). \tag{90}$$

Example 2: For the purpose of comparison we consider the following exact solutions:

$$u(x,t) = x^2 + 2xt + \sin(2\pi x),$$
$$H(x) = 2x - 2 + 4\pi^2 \sin(2\pi x). \tag{91}$$

In Eq. (90) we tentatively disregard the ill-posedness of $f''(x)$, and suppose that the data $f''(x)$ are given exactly. We solve this problem by the OGRSDM and OGRSDM-γ both with $\gamma_0 = 0.1$ and the convergence criterion is $\varepsilon = 0.01$. A

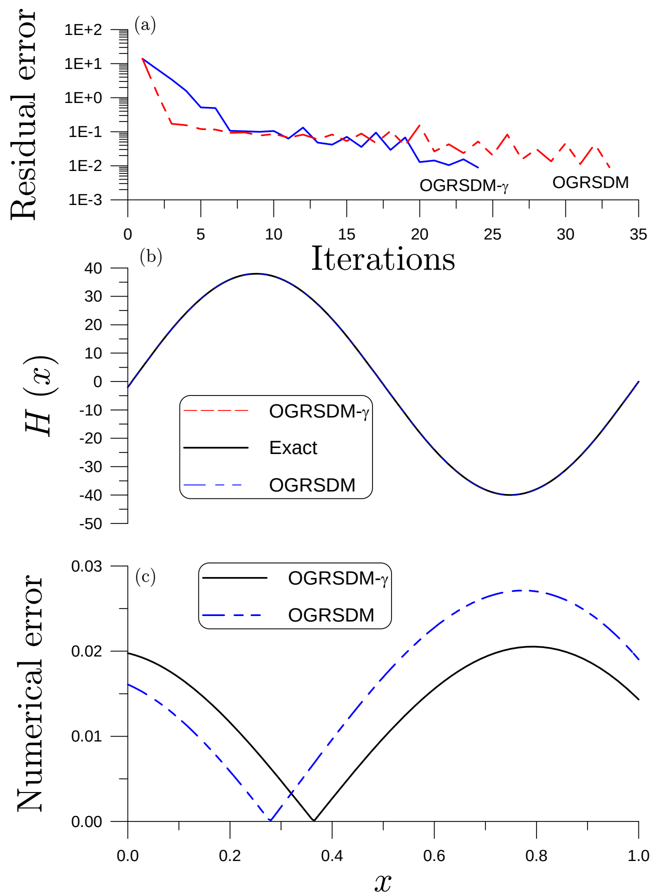

Figure 6: For example 2, (a) comparing the residual errors, (b) comparing the numerical solutions with exact solution, and (c) showing the numerical errors.

random noise with an intensity $\sigma = 0.05$ is added on the data $\dot{q}(t)$. When the OGRSDM is through 33 iterations to find a solution, the OGRSDM-γ only spends 24 iterations, of which the residual errors are shown in Fig. 6(a).

We compare the heat sources recovered by the OGRSDM and OGRSDM-γ with the exact one in Fig. 6(b). As shown in Fig. 6(c), the numerical error of OGRSDM is smaller than 0.0271, and that of OGRSDM-γ is smaller than 0.0205. The iterative algorithms OGRSDM and OGRSDM-γ have provided rather accurate numerical results, even a 5% noise is added on the measured data $\dot{q}(t)$. In Fig. 7(a) we compare the values of a_0 for the OGRSDM and OGRSDM-γ and the value of γ for

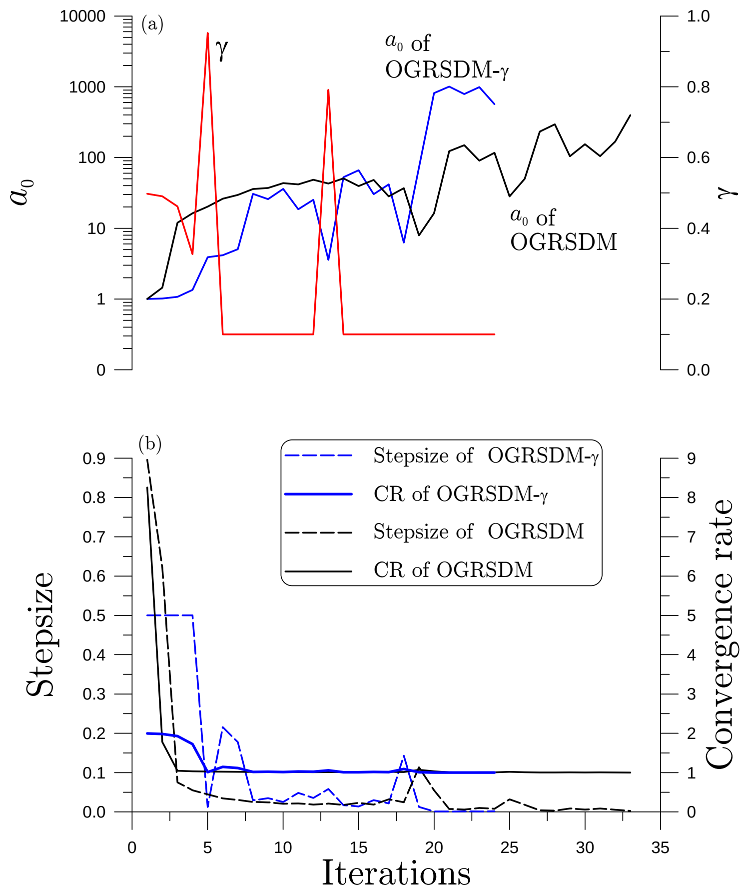

Figure 7: For example 2, (a) comparing the values of a_0 for OGRSDM (black) and OGRSDM-γ (blue), and showing the relaxation parameter of OGRSDM-γ, and (b) comparing the values of stepsize and convergence rate (CR) for OGRSDM (black) and OGRSDM-γ (blue).

OGRSDM-γ. One can appreciate that the alternative use of γ in the OGRSDM-γ can reduce the value of a_0 and accelerate the convergence. From Fig. 7(b) we can observe that the stepsize and the convergence rate (CR) of OGRSDM-γ are larger than that of the OGRSDM besides at the first step. Indeed, in the OGRSDM-γ a new strategy is that under a favorable situation with a smaller a_0, the OGRSDM-γ uses a suitable stepsize $\eta = (1-\gamma)/a_0$ with $\gamma = |a_0/2-1|$, instead of the conservative one $\eta = (1-\gamma_0)/a_0$, which is used in the OGRSDM.

5.4 Inverse Cauchy problems

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

$$\Delta u = u_{rr} + \frac{1}{r}u_r + \frac{1}{r^2}u_{\theta\theta} = 0, \tag{92}$$

$$u(\rho,\theta) = h(\theta), \;\; 0 \le \theta \le \beta_0\pi, \tag{93}$$

$$u_n(\rho,\theta) = g(\theta), \;\; 0 \le \theta \le \beta_0\pi, \tag{94}$$

where $h(\theta)$ and $g(\theta)$ are given functions and $\beta_0 \le 1$. 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. (92)-(94) with the overspecified data on $\Gamma_1 := \{(r,\theta)|r = \rho(\theta),\, 0 \le \theta \le \beta_0\pi\}$.
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 $U(\mathbf{z},\mathbf{s}_j)$:

$$u(\mathbf{z}) = \sum_{j=1}^{n} c_j U(\mathbf{z},\mathbf{s}_j), \;\; \mathbf{s}_j \in \Omega^c. \tag{95}$$

For the Laplace equation (92) we have the fundamental solutions:

$$U(\mathbf{z},\mathbf{s}_j) = \ln r_j, \;\; r_j = \|\mathbf{z}-\mathbf{s}_j\|. \tag{96}$$

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 (93) and (94) on Eq. (95) we can obtain a linear equations system:

$$\mathbf{V}\mathbf{x} = \mathbf{b}_1, \tag{97}$$

where

$$\begin{aligned}
&\mathbf{z}_i = (z_i^1, z_i^2) = (\rho(\theta_i)\cos\theta_i, \rho(\theta_i)\sin\theta_i),\\
&\mathbf{s}_j = (s_j^1, s_j^2) = (R(\theta_j)\cos\theta_j, R(\theta_j)\sin\theta_j),\\
&V_{ij} = \ln\|\mathbf{z}_i - \mathbf{s}_j\|, \;\; \text{if } i \text{ is odd},\\
&V_{ij} = \frac{\eta(\theta_i)}{\|\mathbf{z}_i-\mathbf{s}_j\|^2}\left(\rho(\theta_i) - s_j^1\cos\theta_i - s_j^2\sin\theta_i - \frac{\rho'(\theta_i)}{\rho(\theta_i)}[s_j^1\sin\theta_i - s_j^2\cos\theta_i]\right), \text{if } i \text{ is even},\\
&\mathbf{x} = (c_1,\ldots,c_n)^{\mathrm{T}}, \;\; \mathbf{b}_1 = (h(\theta_1), g(\theta_1), \ldots, h(\theta_m), g(\theta_m))^{\mathrm{T}},
\end{aligned} \tag{98}$$

in which $n = 2m$, and

$$\eta(\theta) = \frac{\rho(\theta)}{\sqrt{\rho^2(\theta) + [\rho'(\theta)]^2}}. \tag{99}$$

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 $R(\theta)$.

Example 3: For the purpose of comparison we consider the following exact solution:

$$u(x,y) = \cos x \cosh y + \sin x \sinh y, \tag{100}$$

defined in a domain with a complex amoeba-like irregular shape as a boundary:

$$\rho(\theta) = \exp(\sin\theta)\sin^2(2\theta) + \exp(\cos\theta)\cos^2(2\theta). \tag{101}$$

Here we fix $\beta_0 = 1$. After imposing the boundary conditions (93) and (94) at m points on Eq. (95) we can obtain a linear equations system. Here we fix $n = 2m = 40$ and take $D = 1.5$ to distribute the source points. The noise being imposed on the measured data h and g is $\sigma = 0.01$.

We solve this problem by the OGRSDM and OGRSDM-γ both with $\gamma_0 = 0.01$ and the convergence criterion is $\varepsilon = 0.01$. When the OGRSDM finds a solution through 316 iterations, the OGRSDM-γ spends 249 iterations, of which the residual errors are shown in Fig. 8(a).

We compare the recovered boundary conditions of $f(\theta)$ computed by the OGRSDM and OGRSDM-γ with the exact one in Fig. 8(b). As shown in Fig. 8(c), the numerical error of OGRSDM is smaller than 0.0883, and that of OGRSDM-γ is smaller than 0.0824. It can be seen that both the OGRSDM and OGRSDM-γ can accurately recover the unknown boundary condition. The result is better than that of Liu (2012g) by using the optimal tri-vector iterative algorithm (OTVIA), which leads to the maximum error being 0.22.

In Fig. 9 we compare the values of a_0 for the OGRSDM and OGRSDM-γ and the value of γ for the OGRSDM-γ. One can appreciate that the alternative use of γ in the OGRSDM-γ indeed can reduce the value of a_0 and accelerate the convergence.

Example 4: For the purpose of comparison we consider another exact solution:

$$u(r,\theta) = r^2\cos(2\theta), \tag{102}$$

defined in a domain with a boundary shape given by

$$\rho(\theta) = \sqrt{10 - 6\cos(2\theta)}. \tag{103}$$

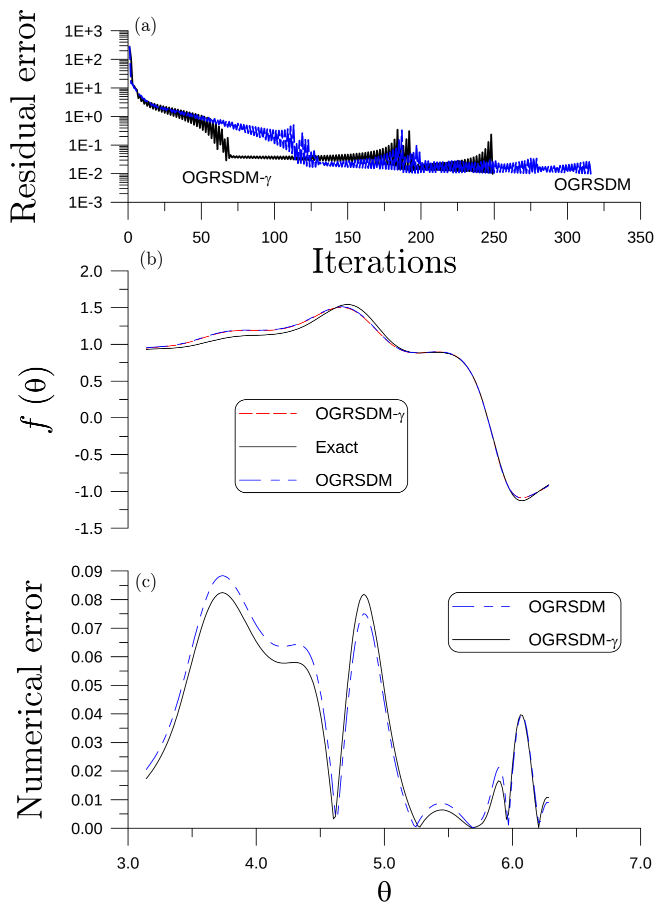

Figure 8: For example 3, (a) comparing the residual errors, (b) comparing the numerical solutions with exact solution, and (c) showing the numerical errors.

We add a random noise with an intensity $\sigma = 1\%$ on the boundary data, and the numerical solution on the boundary $\beta_0\pi < \theta < 2\pi$ with $\beta_0 = 0.4$ is computed by the OGRSDM-γ with $\mathbf{D} = \mathbf{C}^2$ and $\gamma_0 = 0.25$. Under a small convergence criterion $\varepsilon = 10^{-5}$, the OGRSDM-γ converges with 3376 iterations. We take $R = 60$ and $n = 40$ used in the MFS. The residual error is shown in Fig. 10(a), while the values of a_0 and γ are shown in Fig. 10(b).The numerical solution is compared with the exact one in Fig. 10(c), where the maximum error is smaller than 0.145. It indicates that the present OGRSDM-γ is robust against noise, and the required data are parsimonious with $\beta_0 = 0.4$ and under a noise. To our best knowledge, there exist

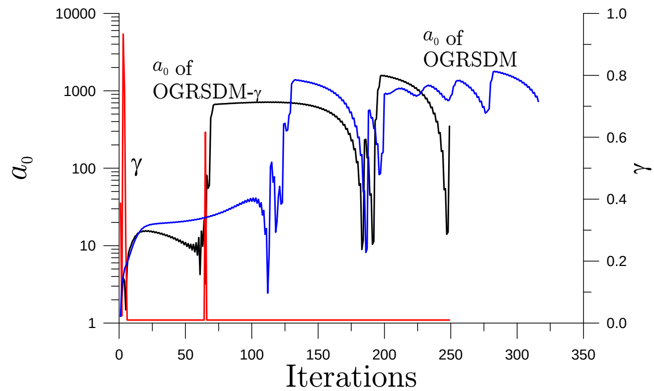

Figure 9: For example 3 comparing the values of a_0 for OGRSDM (black) and OGRSDM-γ (blue), and showing the relaxation parameter of OGRSDM-γ.

no other numerical methods which can treat this type inverse Cauchy problem with $\beta_0 = 0.4$. Previously, Liu (2008b) has used the modified Trefftz method to solve a Cauchy problem with $\beta_0 = 0.5$ on a circular domain.

6 Conclusion

The present paper has introduced an optimal generalization of the steepest descent method in solving ill-posed linear problems. The new method used the optimally preconditioning matrix as a preset before the steepest descent direction. The preconditioner includes two parameters α and γ, where α was optimized by maximizing the convergence speed, while the relaxation parameter γ was computed by $\gamma = |a_0/2-1|$ under a switching criterion $a_0 < 4$, such that γ is either using the specified value γ_0 or using a value computed from the above formula, depending on the value of a_0. In doing so, we have developed a new strategy in the OGRSDM-γ that under a favorable situation with a smaller a_0, the OGRSDM-γ used a better stepsize $\eta = (1-\gamma)/a_0$ with $\gamma = |a_0/2-1|$, instead of the original stepsize $\eta = (1-\gamma_0)/a_0$. It is clever that when the switch is turned-on, by using the derived formula of $\gamma = |a_0/2-1|$ it can pull back the iterative orbit to the **fast manifold**. Several numerical examples explored the efficiency by designing such a switching formula for the computation of the relaxation parameter. The present OGRSDM and OGRSDM-γ have a better computational efficiency and accuracy, which was verified by solving three well-known ill-posed linear inverse problems.

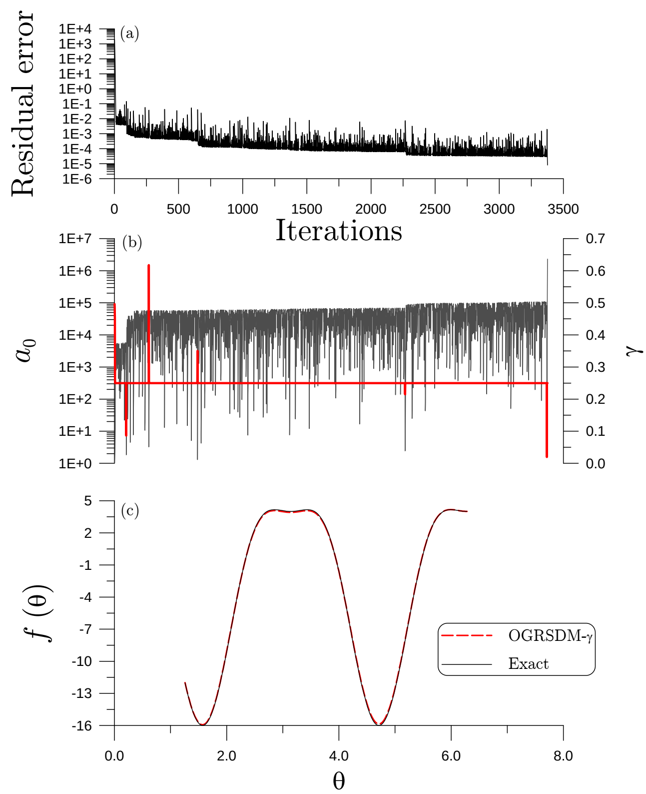

Figure 10: For example 4, (a) showing the residual error, (b) the values of a_0 (black) and γ (red) for OGRSDM-γ, and (c) comparing the numerical solution with the exact solution

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