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Iterated Tikhonov regularization with a general penalty term

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SUMMARY

Tikhonov regularization is one of the most popular approaches to solving linear discrete ill-posed problems. The choice of regularization matrix may significantly affect the quality of the computed solution. When the regularization matrix is the identity, iterated Tikhonov regularization can yield computed approximate solutions of higher quality than (standard) Tikhonov regularization. This paper provides an analysis of iterated Tikhonov regularization with a regularization matrix different from the identity. Computed examples illustrate the performance this method. Copyright © John Wiley & Sons, Ltd.

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1. INTRODUCTION

Many applications in physics and engineering lead to linear least-squares problems of the form

$$\min_{\mathbf{x}\in\mathbb{R}^{d_2}} \|A\mathbf{x}-\mathbf{b}^\delta\|, \quad A\in\mathbb{R}^{d_1\times d_2}, \quad \mathbf{b}^\delta\in\mathbb{R}^{d_1}, \tag{1}$$

where the vector $\mathbf{b}^\delta$ represents measured data that is contaminated by an unknown error $\mathbf{e}\in\mathbb{R}^{d_1}$ of norm bounded by $\delta>0$, and the matrix A is of ill-determined rank, i.e., its singular values decay gradually to zero without a significant gap. Least-squares problems with a matrix of this kind are commonly referred to as discrete ill-posed problems. They arise, for instance, from the discretization of linear ill-posed problems; see [1, 2] for discussions on ill-posed and discrete ill-posed problems.

Let $\mathbf{b}$ denote the unknown error-free vector associated with $\mathbf{b}^\delta$. Then

$$\mathbf{b}^\delta = \mathbf{b}+\mathbf{e}, \qquad \|\mathbf{e}\|\le\delta. \tag{2}$$

Here and throughout this paper, $\|\cdot\|$ denotes the Euclidean vector norm or spectral matrix norm.

Assuming that $\mathbf{b}$ is attainable, we would like to determine an accurate approximation of the minimal norm solution $\mathbf{x}^\dagger := A^\dagger\mathbf{b}$ of the error-free least-squares problem associated with (1). Here $A^\dagger$ denotes the Moore–Penrose pseudoinverse. Due to the clustering of the singular values of A at

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the origin and the error in $\mathbf{b}^\delta$, the solution $A^\dagger\mathbf{b}^\delta$ of (1) generally is not a meaningful approximation of $\mathbf{x}^\dagger$. This difficulty can be remedied by replacing the minimization problem (1) by a nearby problem whose solution is less sensitive to the error in $\mathbf{b}^\delta$. This replacement is commonly referred to as regularization [1]. One of the most popular regularization methods is due to Tikhonov, which in its simplest form replaces the least-squares problem (1) by the penalized minimization problem

$$\min_{\mathbf{x}\in\mathbb{R}^{d_2}}\{\left\|A\mathbf{x}-\mathbf{b}^\delta\right\|^2+\alpha\left\|\mathbf{x}-\mathbf{x}_0\right\|^2\}. \tag{3}$$

Here $\alpha>0$ is a regularization parameter whose value determines how sensitive the solution of (3) is to the error $\mathbf{e}$ in $\mathbf{b}^\delta$ and how close the solution is to the desired vector $\mathbf{x}^\dagger$. The vector $\mathbf{x}_0\in\mathbb{R}^{d_2}$ is an available approximation of $\mathbf{x}^\dagger$. It may be set to zero if no approximation of $\mathbf{x}^\dagger$ is known; see, e.g., [1, 2] for discussions on Tikhonov regularization.

It is well known that it often is possible to improve the quality of the approximation of $\mathbf{x}^\dagger$ determined by Tikhonov regularization by replacing the Tikhonov minimization problem (3) by

$$\min_{\mathbf{x}\in\mathbb{R}^{d_2}}\{\left\|A\mathbf{x}-\mathbf{b}^\delta\right\|^2+\alpha\left\|L(\mathbf{x}-\mathbf{x}_0)\right\|^2\}, \tag{4}$$

where $L\in\mathbb{R}^{d_3\times d_2}$ is a suitable regularization matrix. Let $\mathcal{N}(L)$ and $\mathcal{R}(L)$ denote the null space and the range of L, respectively. We will assume that L is chosen so that

$$\mathcal{N}(L)\cap\mathcal{N}(A)=\{\mathbf{0}\}. \tag{5}$$

Then (4) has a unique solution $\mathbf{x}_\alpha$ for any $\alpha>0$. The minimization problem (3) is commonly referred to as Tikhonov regularization in *standard form*, while (4) is referred to as Tikhonov regularization in *general form*. Discussions on and illustrations of the performance of Tikhonov regularization in general form can be found in, e.g., [2, 3, 4, 5].

We first consider the minimization problem (3), which we express as

$$\min_{\mathbf{h}\in\mathbb{R}^{d_2}}\{\left\|A\mathbf{h}-\mathbf{r}_0\right\|^2+\alpha\left\|\mathbf{h}\right\|^2\},$$

where

$$\mathbf{r}_0=\mathbf{b}^\delta-A\mathbf{x}_0,\qquad \mathbf{h}=\mathbf{x}-\mathbf{x_0}.$$

Thus, $\mathbf{h}$ provides an approximation of the error $\mathbf{x}^\dagger-\mathbf{x}_0$ and, for a suitable choice of $\alpha>0$, generally, an improved approximation of $\mathbf{x}^\dagger$ is given by

$$\mathbf{x}_1=\mathbf{x}_0+\mathbf{h}.$$

Repeated application of this refinement strategy defines the *iterated Tikhonov method* [1]. Given $\mathbf{x}_0\in\mathbb{R}^n$, we carry out the following steps:

for $k=0,1,\dots$ do

1. Compute $\mathbf{r}_k=\mathbf{b}^\delta-A\mathbf{x}_k$
2. Solve $\min_{\mathbf{h}\in\mathbb{R}^{d_2}}\{\left\|A\mathbf{h}-\mathbf{r}_k\right\|^2+\alpha_k\left\|\mathbf{h}\right\|^2\}$ to obtain $\mathbf{h}_k$
3. Update $\mathbf{x}_{k+1}=\mathbf{x}_k+\mathbf{h}_k$

where $\alpha_0,\alpha_1,\dots$ denotes a sequence of positive regularization parameters. We will comment on their choice below.

The iterations for the iterated Tikhonov method can be expressed compactly in the form

$$\mathbf{x}_{k+1}=\mathbf{x}_k+(A^tA+\alpha_kI)^{-1}A^t(\mathbf{b}^\delta-A\mathbf{x}_k),\qquad k=0,1,\dots, \tag{6}$$

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where the superscript ^{t} stands for transposition and I denotes the identity matrix. The iterations can be terminated with the aid of the *discrepancy principle*, which prescribes that k be increased until

$$\|\mathbf{r}_{k+1}\| \le \tau\delta \tag{7}$$

holds. Here $\tau > 1$ is a user-supplied constant independent of δ; see, e.g., [1, 2] for discussions on the discrepancy principle. Its application requires that the least-squares problem (1) with $\mathbf{b}^\delta$ replaced by the associated error-free vector $\mathbf{b}$ be consistent.

The choice of α_k in the iterated Tikhonov method is important and many strategies have been proposed in the literature; see [6] for a recent discussion. If $\alpha_k = \alpha$ is independent of k, then the iterative method is said to be *stationary*, otherwise it is *non-stationary*. In many applications non-stationary iterated Tikhonov regularization has been found to give more accurate approximations of $\mathbf{x}^\dagger$ and/or a faster convergence than stationary iterated Tikhonov regularization. A common choice of regularization parameters for non-stationary iterated Tikhonov methods is the geometric sequence

$$\alpha_k = \alpha_0 q^k, \qquad \alpha_0 > 0, \quad 0 < q < 1, \qquad k = 0, 1, \dots \,. \tag{8}$$

This choice is studied in [7, 8].

Available analyses of iterated Tikhonov regularization only treat the case when L is the identity [6, 7, 8, 9], i.e., the iteration (6). However, computed results reported in [10, 11] show that iterative application of (4) with $L \neq I$ can give better approximations of $\mathbf{x}^\dagger$ than (6). Similarly, extending an approximate version of (6) proposed in [12], the results in [13] show that the computed approximations of $\mathbf{x}^\dagger$ can be improved by choosing a regularization matrix different from the identity. Nevertheless, to the best of our knowledge no detailed analysis of iterated Tikhonov regularization

$$\mathbf{x}_{k+1} = \mathbf{x}_k + (A^tA + \alpha_k L^tL)^{-1}A^t(\mathbf{b}^\delta - A\mathbf{x}_k), \qquad k = 0, 1, \dots, \tag{9}$$

with L a fairly general regularization matrix that satisfies (5) is available. It is the aim of this paper to provide such an analysis and to show that, for suitable choices of L, the iteration (9) can give approximations of $\mathbf{x}^\dagger$ of significantly higher quality than the iterations (6). We show that (9) defines a regularization method when the iterations are terminated with the discrepancy principle (7). Our analysis is first carried out for the stationary iterated Tikhonov method with A and L square matrices, and subsequently extended to rectangular matrices and non-stationary iterated Tikhonov regularization.

This paper is organized as follows: Section 2 uses the generalized singular value decomposition of the matrix pair $\{A, L\}$ to derive some results which are needed in the following. The iterated Tikhonov method with a general regularization matrix L is discussed in Section 3. We describe an algorithm and discuss properties of the iterates generated. A few computed examples that illustrate the performance of iterated Tikhonov regularization are presented in Section 4, and concluding remarks can be found in Section 5.

2. STANDARD TIKHONOV REGULARIZATION IN GENERAL FORM

Assume that A and L are square matrices, i.e., $d_1 = d_2 = d_3 = d$, and introduce the generalized singular value decomposition (GSVD) of the matrix pair $\{A, L\}$,

$$A = U\Sigma Y^t, \quad L = V\Lambda Y^t, \tag{10}$$

where $U, V \in \mathbb{R}^{d\times d}$ are orthogonal matrices, $\Sigma = \mathrm{diag}[\sigma_1, \dots, \sigma_d] \in \mathbb{R}^{d\times d}$ and $\Lambda = \mathrm{diag}[\lambda_1, \dots, \lambda_d] \in \mathbb{R}^{d\times d}$ are diagonal matrices, and the matrix $Y \in \mathbb{R}^{d\times d}$ is non-singular. It follows from (5) that

$$\sigma_j = 0 \Rightarrow \lambda_j \neq 0 \quad \text{and} \quad \lambda_j = 0 \Rightarrow \sigma_j \neq 0. \tag{11}$$

Due to (5), the minimization problem

$$\min_{\mathbf{x}\in\mathbb{R}^d}\{\left\|A\mathbf{x} - \mathbf{b}^\delta\right\|^2 + \alpha\left\|L\mathbf{x}\right\|^2\}$$

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has the unique solution

$$\mathbf{x}_\alpha = \left(A^tA + \alpha L^tL\right)^{-1} A^t\mathbf{b}^\delta. \tag{12}$$

Substituting the factorizations (10) into (12), we get

$$\begin{aligned}\mathbf{x}_\alpha &= \left(Y\Sigma U^tU\Sigma Y^t + \alpha Y\Lambda V^tV\Lambda Y^t\right)^{-1} Y\Sigma U^t\mathbf{b}^\delta\\ &= Y^{-t}\left(\Sigma^2 + \alpha\Lambda^2\right)^{-1}\Sigma U^t\mathbf{b}^\delta\\ &= Y^{-t}\left(\Sigma^2 + \alpha\Lambda^2\right)^{-1}\Sigma\hat{\mathbf{b}},\end{aligned}$$

where $\hat{\mathbf{b}} = [\hat{b}_1, \ldots, \hat{b}_d]^t = U^t\mathbf{b}^\delta$. Assume that $\lambda_j = 0$ for $1 \le j \le l$, and $\lambda_j \neq 0$ for $l < j \le d$. Note that, due to (11), the ratios $\frac{1}{\sigma_j}$, $1 \le j \le l$, are well defined. Then we have

$$\begin{aligned}\mathbf{x}_\alpha &= \sum_{j=1}^{d} \tilde{y}_j \frac{\sigma_j}{\sigma_j^2 + \alpha\lambda_j^2}\hat{b}_j\\ &= \sum_{j=1}^{l} \tilde{y}_j \frac{1}{\sigma_j}\hat{b}_j + \sum_{j=l+1}^{d} \tilde{y}_j \frac{\sigma_j}{\sigma_j^2 + \alpha\lambda_j^2}\hat{b}_j\\ &= \sum_{j=1}^{l} \tilde{y}_j \frac{1}{\sigma_j}\hat{b}_j + \sum_{j=l+1}^{d} \tilde{y}_j \frac{\sigma_j/\lambda_j}{(\sigma_j/\lambda_j)^2 + \alpha}\frac{1}{\lambda_j}\hat{b}_j.\end{aligned} \tag{13}$$

Let us give some definitions that are going to be useful in the following. Introduce the matrix

$$A_{\mathcal{N}(L)}^{-1} = Y^{-t}\begin{pmatrix} 1/\sigma_1 & & & & & & \\ & 1/\sigma_2 & & & & & \\ & & \ddots & & & & \\ & & & 1/\sigma_r & & & \\ & & & & 0 & & \\ & & & & & \ddots & \\ & & & & & & 0 \end{pmatrix} U^t = Y^{-t}\Sigma^\dagger(I - \Lambda^\dagger\Lambda)U^t, \tag{14}$$

where $r = \min\{l, \mathrm{rank}(A)\}$ and

$$\Lambda^\dagger = \begin{pmatrix} 0 & & & & & \\ & \ddots & & & & \\ & & 0 & & & \\ & & & 1/\lambda_{l+1} & & \\ & & & & \ddots & \\ & & & & & 1/\lambda_d \end{pmatrix}$$

is the pseudoinverse of Λ. Also define

$$\bar{L} = Y^{-t}\Lambda^\dagger V^t. \tag{15}$$

Let $\Gamma = \mathrm{diag}[\gamma_1, \ldots, \gamma_d]$ with $\gamma_j = 0$ for $1 \le j \le l$ and $\gamma_j = \frac{\sigma_j}{\lambda_j}$ for $l < j \le d$. Introduce

$$C = U\Gamma V^t. \tag{16}$$

Since the matrices U and V are orthogonal, it follows that (16) is the singular value decomposition (SVD) of C, possibly with the entries of Γ ordered in a non-standard fashion, i.e., it is not assured that $\gamma_j \geq \gamma_{j+1}$ for all j as in the standard SVD. Combining (14)–(16) with (13), we now can express the solution of (12) as

$$\mathbf{x}_\alpha = A_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta + \bar{L}\left(C^tC + \alpha I\right)^{-1} C^t\mathbf{b}^\delta.$$

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3. ITERATED TIKHONOV REGULARIZATION WITH A GENERAL PENALTY TERM

The following algorithm extends iterated Tikhonov regularization with $L = I$ in the stationary case, i.e., with $\alpha_k = \alpha$ for all k, by allowing a fairly general regularization matrix L. The algorithm does not require the matrices A and L to be square.

Algorithm 1 (GIT)
Let $A \in \mathbb{R}^{d_1 \times d_2}$ and $\mathbf{b}^\delta \in \mathbb{R}^{d_1}$, and let the regularization matrix $L \in \mathbb{R}^{d_3 \times d_2}$ satisfy (5). Assume that $\delta > 0$ is large enough so that (2) holds and fix $\tau > 1$ independently of δ. Let $\alpha > 0$ and let $\mathbf{x}_0 \in \mathbb{R}^{d_2}$ be an available initial approximation of $\mathbf{x}^\dagger$. Compute

$$
\begin{aligned}
&\text{for } k = 0, 1, \dots \\
&\quad \mathbf{r}_k = \mathbf{b}^\delta - A\mathbf{x}_k \\
&\quad \text{if } \|\mathbf{r}_k\| < \tau\delta \text{ exit} \\
&\quad \mathbf{x}_{k+1} = \mathbf{x}_k + \left(A^t A + \alpha L^t L\right)^{-1} A^t \mathbf{r}_k \\
&\text{end}
\end{aligned}
$$

In the special case when L is the identity matrix, Algorithm 1 simplifies to the iterations (6) terminated by the discrepancy principle (7). In our analysis of Algorithm 1, we first consider the situation when A and L are square matrices. Later, in Subsection 3.2, we extend the analysis to more general matrices A and L. Finally, in Subsection 3.3, we consider non-stationary sequences of regularization parameters $\alpha_0, \alpha_1, \alpha_2, \dots$.

3.1. *Convergence analysis for square matrices A and L*

Let $d = d_1 = d_2 = d_3$. In this subsection we will show that the iterates $\mathbf{x}_k$ determined by Algorithm 1 without termination by the discrepancy principle converge to the solution of (1). However, as we pointed out in Section 1, the solution of (1) is contaminated by propagated error and therefore generally not useful. Typically, a much better approximation of $\mathbf{x}^\dagger$ can be determined by early termination of the iterations with the aid of the discrepancy principle as in Algorithm 1. We will show that Algorithm 1 defines an iterative regularization method.

To show convergence and the regularization property of Algorithm 1, we employ a *divide et impera* approach. We set $\mathbf{x}_0 = \mathbf{0}$ in order to simplify the proofs. Consider the iterates

$$
\begin{cases}
\mathbf{x}_0 = \mathbf{0}, \\
\mathbf{x}_{k+1} = \mathbf{x}_k + (A^t A + \alpha L^t L)^{-1} A^t \mathbf{r}_k,
\end{cases}
$$

where $\mathbf{r}_k = \mathbf{b}^\delta - A\mathbf{x}_k$ is the residual at step k. Using the expression (13), we get that

$$
\begin{aligned}
\mathbf{x}_{k+1} &= \mathbf{x}_k + A^{-1}_{\mathcal{N}(L)} \mathbf{r}_k + \bar{L}\left(C^t C + \alpha I\right)^{-1} C^t \mathbf{r}_k \\
&= \sum_{i=0}^{k} A^{-1}_{\mathcal{N}(L)} \mathbf{r}_i + \sum_{i=0}^{k} \bar{L}\left(C^t C + \alpha I\right)^{-1} C^t \mathbf{r}_i .
\end{aligned}
$$

We will show convergence of the two sums

$$
\mathbf{x}^{(0)}_{k+1} = \sum_{i=0}^{k} A^{-1}_{\mathcal{N}(L)} \mathbf{r}_i, \tag{17}
$$

$$
\mathbf{x}^{\perp}_{k+1} = \bar{L} \sum_{i=0}^{k} \left(C^t C + \alpha I\right)^{-1} C^t \mathbf{r}_i \tag{18}
$$

for increasing k separately.

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Proposition 1
Assume $d = d_1 = d_2 = d_3$, let $\mathbf{x}_k^{(0)}$ be defined in (17), and set $\mathbf{x}_0 = \mathbf{0}$. Then

$$\mathbf{x}_k^{(0)} = A_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta \text{ for } k \geq 1.$$

Proof
Since $\mathbf{x}_0 = \mathbf{0}$, we immediately have that

$$\mathbf{x}_1^{(0)} = A_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta.$$

It remains to be shown that $\mathbf{x}_k^{(0)} = A_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta$ for all $k \geq 2$. We proceed by induction. Let $k \geq 1$ and suppose that $\mathbf{x}_k^{(0)} = A_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta$. Then we need to show that $\mathbf{x}_{k+1}^{(0)} = A_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta$. We have

$$\begin{aligned}
\mathbf{x}_{k+1}^{(0)} &= \mathbf{x}_k^{(0)} + A_{\mathcal{N}(L)}^{-1}(\mathbf{b}^\delta - A\mathbf{x}_k) \\
&= A_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta + A_{\mathcal{N}(L)}^{-1}(\mathbf{b}^\delta - A(\mathbf{x}_k^{(0)} + \mathbf{x}_k^{\perp})) \\
&= A_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta + A_{\mathcal{N}(L)}^{-1}(\mathbf{b}^\delta - AA_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta - A\mathbf{x}_k^{\perp}).
\end{aligned}$$

If we show that $A_{\mathcal{N}(L)}^{-1}(\mathbf{b}^\delta - AA_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta) = A_{\mathcal{N}(L)}^{-1}A\mathbf{x}_k^{\perp} = \mathbf{0}$, then the proposition follows. We have that

$$\begin{aligned}
&A_{\mathcal{N}(L)}^{-1}(\mathbf{b}^\delta - AA_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta) = (A_{\mathcal{N}(L)}^{-1} - A_{\mathcal{N}(L)}^{-1}AA_{\mathcal{N}(L)}^{-1})\mathbf{b}^\delta \\
&= (Y^{-t}\Sigma^\dagger(I - \Lambda^\dagger\Lambda)U^t - Y^{-t}\Sigma^\dagger(I - \Lambda^\dagger\Lambda)U^tU\Sigma Y^tY^{-t}\Sigma^\dagger(I - \Lambda^\dagger\Lambda)U^t)\mathbf{b}^\delta \\
&= Y^{-t}(\Sigma^\dagger(I - \Lambda^\dagger\Lambda) - \Sigma^\dagger(I - \Lambda^\dagger\Lambda)\Sigma\Sigma^\dagger(I - \Lambda^\dagger\Lambda))U^t\mathbf{b}^\delta \\
&= Y^{-t}(\Sigma^\dagger(I - \Lambda^\dagger\Lambda) - \Sigma^\dagger\Sigma\Sigma^\dagger(I - \Lambda^\dagger\Lambda)(I - \Lambda^\dagger\Lambda))U^t\mathbf{b}^\delta \\
&= Y^{-t}(\Sigma^\dagger(I - \Lambda^\dagger\Lambda) - \Sigma^\dagger(I - \Lambda^\dagger\Lambda))U^t\mathbf{b}^\delta = \mathbf{0},
\end{aligned}$$

where we have used the facts that diagonal matrices commute, that $\Sigma^\dagger\Sigma\Sigma^\dagger = \Sigma^\dagger$, and that $(I - \Lambda^\dagger\Lambda)(I - \Lambda^\dagger\Lambda) = (I - \Lambda^\dagger\Lambda)$, since $(I - \Lambda^\dagger\Lambda)$ is an orthogonal projector.

Turning to $A_{\mathcal{N}(L)}^{-1}A\mathbf{x}_k^{\perp}$, we will show that $A_{\mathcal{N}(L)}^{-1}A\bar{L} = 0$. We get

$$\begin{aligned}
A_{\mathcal{N}(L)}^{-1}A\bar{L} &= Y^{-t}\Sigma^\dagger(I - \Lambda^\dagger\Lambda)U^tU\Sigma Y^tY^{-t}\Lambda^\dagger V^t \\
&= Y^{-t}\Sigma^\dagger\Sigma(I - \Lambda^\dagger\Lambda)\Lambda^\dagger V^t \\
&= Y^{-t}\Sigma^\dagger\Sigma(\Lambda^\dagger - \Lambda^\dagger\Lambda\Lambda^\dagger)V^t \\
&= Y^{-t}\Sigma^\dagger\Sigma(\Lambda^\dagger - \Lambda^\dagger)V^t = 0.
\end{aligned}$$

It follows that $A_{\mathcal{N}(L)}^{-1}A\mathbf{x}_k^{\perp} = \mathbf{0}$ by induction because

$$A_{\mathcal{N}(L)}^{-1}A\mathbf{x}_k^{\perp} = A_{\mathcal{N}(L)}^{-1}A\mathbf{x}_{k-1}^{\perp} + A_{\mathcal{N}(L)}^{-1}A\bar{L}(C^tC + \alpha I)^{-1}C^t(\mathbf{b}^\delta - A\mathbf{x}_k),$$

which concludes the proof. □

Proposition 2
Let $d = d_1 = d_2 = d_3$ and assume that (5) holds. Let $\mathbf{x}_k^{\perp}$ be defined in (18) and set $\mathbf{x}_0 = \mathbf{0}$. Then

$$\mathbf{x}_k^{\perp} \to \bar{L}C^\dagger\bar{\mathbf{b}}^\delta \text{ as } k \to \infty,$$

where

$$\bar{\mathbf{b}}^\delta = U\Lambda^\dagger\Lambda U^t\mathbf{b}^\delta.$$

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Proof
Consider the sequence $\{\mathbf{x}_k^\perp\}_{k=1}^\infty$. We would like to show that this sequence can be determined by application of standard iterated Tikhonov regularization to some linear system of equations. The convergence then will follow from available results for iterative Tikhonov regularization with regularization matrix $L = I$. First recall the expression for $\mathbf{x}_{k+1}^\perp$,

$$\mathbf{x}_{k+1}^\perp = \mathbf{x}_k^\perp + \bar{L}(C^tC + \alpha I)^{-1}C^t(\mathbf{b}^\delta - A\mathbf{x}_k).$$

To transform this iteration to (standard) iterated Tikhonov iterations, we introduce

$$\tilde{\mathbf{h}}_k = (C^tC + \alpha I)^{-1}C^t(\mathbf{b}^\delta - A\mathbf{x}_k), \tag{19}$$

such that

$$\mathbf{x}_{k+1}^\perp = \mathbf{x}_k^\perp + \bar{L}\tilde{\mathbf{h}}_k. \tag{20}$$

Inserting the factorizations (10) and (16) of A and C into (19) yields

$$\tilde{\mathbf{h}}_k = V(\Gamma^2 + \alpha I)^{-1}\Gamma U^t(\mathbf{b}^\delta - U\Sigma Y^t\mathbf{x}_k) = V(\Gamma^2 + \alpha I)^{-1}\Gamma(U^t\mathbf{b}^\delta - \Sigma Y^t\mathbf{x}_k).$$

We have

$$\Gamma\Sigma = \Gamma\Gamma\Lambda,$$

because both the left-hand and right-hand sides are diagonal matrices whose first l components vanish, and the remaining components are of the form σ_j^2/λ_j for $l < j \leq d$. Thus, we obtain

$$\tilde{\mathbf{h}}_k = V(\Gamma^2 + \alpha I)^{-1}\Gamma(U^tb - \Gamma\Lambda Y^t\mathbf{x}_k).$$

Define

$$\bar{\mathbf{b}}^\delta = U\Lambda^\dagger\Lambda U^t\mathbf{b}^\delta$$

and

$$\bar{\mathbf{x}}_k = L\mathbf{x}_k,$$

and consider

$$\bar{\mathbf{h}}_k = (C^tC + \alpha I)^{-1}C^t(\bar{\mathbf{b}}^\delta - C\bar{\mathbf{x}}_k).$$

We will show that $\bar{\mathbf{h}}_k = \tilde{\mathbf{h}}_k$. Substituting the factorizations (16) and (10) of C and L into the above expression, we get

$$\begin{aligned}\bar{\mathbf{h}}_k &= V(\Gamma^2 + \alpha I)^{-1}V^tV\Gamma U^t(U\Lambda^\dagger\Lambda U^t\mathbf{b}^\delta - U\Gamma V^tV\Lambda Y^t\mathbf{x}_k)\\ &= V(\Gamma^2 + \alpha I)^{-1}\Gamma(U^t\mathbf{b}^\delta - \Gamma\Lambda Y^t\mathbf{x}_k) = \tilde{\mathbf{h}}_k,\end{aligned}$$

where in the last step we used the fact that $\Gamma\Lambda^\dagger\Lambda = \Gamma$. Replacing $\tilde{\mathbf{h}}_k$ by $\bar{\mathbf{h}}_k$ in (20), we obtain

$$\mathbf{x}_{k+1}^\perp = \mathbf{x}_k^\perp + \bar{L}\bar{\mathbf{h}}_k = \mathbf{x}_k^\perp + \bar{L}(C^tC + \alpha I)^{-1}C^t(\bar{\mathbf{b}}^\delta - CL\mathbf{x}_k).$$

Since $\mathbf{x}_0 = \mathbf{0}$, we have

$$\mathbf{x}_{k+1}^\perp = \bar{L}\sum_{i=0}^{k}(C^tC + \alpha I)^{-1}C^t(\bar{\mathbf{b}}^\delta - CL\mathbf{x}_i).$$

We now show that the sum in the right-hand side, namely

$$\tilde{\mathbf{x}}_{k+1} = \sum_{i=0}^{k}(C^tC + \alpha I)^{-1}C^t(\bar{\mathbf{b}}^\delta - CL\mathbf{x}_i)$$

is the approximate solution computed by $k+1$ iterations of standard iterated Tikhonov iteration applied to the linear system of equations

$$C\mathbf{x} = \bar{\mathbf{b}}^\delta. \tag{21}$$

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We have

$$\tilde{\mathbf{x}}_{k+1} = \tilde{\mathbf{x}}_k + (C^tC + \alpha I)^{-1}C^t(\bar{\mathbf{b}}^\delta - CL\mathbf{x}_k).$$

Therefore, if we establish that $L\mathbf{x}_k = \tilde{\mathbf{x}}_k$ for all k, then we are done. We show this result by induction. For $k = 0$ it is trivial since $\mathbf{x}_0 = \mathbf{0}$. Suppose that $\tilde{\mathbf{x}}_k = L\mathbf{x}_k$. We would like to show that $\tilde{\mathbf{x}}_{k+1} = L\mathbf{x}_{k+1}$. Applying L to $\mathbf{x}_{k+1}$ yields

$$\begin{aligned}
L\mathbf{x}_{k+1} &= L\mathbf{x}_k + LA^{-1}_{\mathcal{N}(L)}\mathbf{r}_k + L\bar{L}(C^tC + \alpha I)^{-1}C^t(\mathbf{b}^\delta - A\mathbf{x}_k)\\
&\stackrel{(a)}{=} \tilde{\mathbf{x}}_k + 0 + L\bar{L}(C^tC + \alpha I)^{-1}C^t(\mathbf{b}^\delta - A\mathbf{x}_k)\\
&\stackrel{(b)}{=} \tilde{\mathbf{x}}_k + L\bar{L}(C^tC + \alpha I)^{-1}C^t(\bar{\mathbf{b}}^\delta - CL\mathbf{x}_k)\\
&= \tilde{\mathbf{x}}_k + V\Lambda^\dagger Y^tY^{-t}\Lambda V^tV(\Gamma^2 + \alpha I)^{-1}\Gamma U^t(\bar{\mathbf{b}}^\delta - CL\mathbf{x}_k)\\
&= \tilde{\mathbf{x}}_k + V\Lambda^\dagger\Lambda(\Gamma^2 + \alpha I)^{-1}\Gamma U^t(\bar{\mathbf{b}}^\delta - CL\mathbf{x}_k)\\
&\stackrel{(c)}{=} \tilde{\mathbf{x}}_k + V(\Gamma^2 + \alpha I)^{-1}\Gamma U^t(\bar{\mathbf{b}}^\delta - CL\mathbf{x}_k)\\
&= \tilde{\mathbf{x}}_k + (C^tC + \alpha I)^{-1}C^t(\bar{\mathbf{b}}^\delta - CL\mathbf{x}_k) = \tilde{\mathbf{x}}_{k+1},
\end{aligned}$$

where equality (a) is due to the fact that $A^{-1}_{\mathcal{N}(L)}$ annihilates the component of $\mathbf{r}_k = \mathbf{b}^\delta - A\mathbf{x}_k$ in the complement of $\mathcal{N}(L)$, (b) is obtained by using the fact, shown above, that $\tilde{\mathbf{h}}_k = \bar{\mathbf{h}}_k$, and (c) follows from $\Lambda^\dagger\Lambda\Gamma = \Gamma$.

We have shown that the $\tilde{\mathbf{x}}_k$ are iterates determined by the (standard) iterated Tikhonov method applied to the linear system of equations (21) and thus it follows that

$$\tilde{\mathbf{x}}_k \to C^\dagger\bar{\mathbf{b}}^\delta \text{ as } k \to \infty,$$

due to the convergence of the iterated Tikhonov method [1]. By continuity of $\bar{L}$, we have that

$$\mathbf{x}_k^\perp \to \bar{L}C^\dagger\bar{\mathbf{b}}^\delta \text{ as } k \to \infty,$$

which concludes the proof. □

Introduce the matrix

$$A^{(\dagger)} = Y^{-t}\Sigma^\dagger U^t.$$

Theorem 3
Let $d = d_1 = d_2 = d_3$ and assume that (5) holds. Let $\mathbf{x}_0 = \mathbf{0}$. Then the iterates determined by Algorithm 1 converge to $A^{(\dagger)}\mathbf{b}^\delta$. Moreover, if $\mathbf{b}^\delta \in \mathcal{R}(A)$, then $AA^{(\dagger)}\mathbf{b}^\delta = \mathbf{b}^\delta$.

Proof
From Propositions 1 and 2, we have

$$\mathbf{x}_k = \mathbf{x}_k^{(0)} + \mathbf{x}_k^\perp \to A^{-1}_{\mathcal{N}(L)}\mathbf{b}^\delta + \bar{L}C^\dagger\bar{\mathbf{b}}^\delta = \mathbf{x}_\infty \text{ as } k \to \infty.$$

Using the definitions (14), (15), and (16), we obtain

$$\begin{aligned}
\mathbf{x}_\infty &= Y^{-t}\Sigma^\dagger(I - \Lambda^\dagger\Lambda)U^t\mathbf{b}^\delta + Y^{-t}\Lambda^\dagger V^tV\Gamma^\dagger U^tU\Lambda^\dagger\Lambda U^t\mathbf{b}^\delta\\
&= Y^{-t}\left(\Sigma^\dagger(I - \Lambda^\dagger\Lambda) + \Lambda^\dagger\Gamma^\dagger\Lambda^\dagger\Lambda\right)U^t\mathbf{b}^\delta\\
&= Y^{-t}\left(\Sigma^\dagger(I - \Lambda^\dagger\Lambda) + \Lambda^\dagger\Gamma^\dagger\right)U^t\mathbf{b}^\delta\\
&= Y^{-t}\left(\Sigma^\dagger(I - \Lambda^\dagger\Lambda) + \Lambda^\dagger\Lambda\Sigma^\dagger\right)U^t\mathbf{b}^\delta\\
&= Y^{-t}\Sigma^\dagger U^t\mathbf{b}^\delta,
\end{aligned}$$

where we have used the fact that diagonal matrices commute and $\Lambda^\dagger\Gamma^\dagger = \Lambda^\dagger\Lambda\Sigma^\dagger$.

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What is left to prove is that if $\mathbf{b}^\delta \in \mathcal{R}(A)$, then $AA^{(\dagger)}\mathbf{b}^\delta = \mathbf{b}^\delta$, which is straightforward. Since $\mathbf{b}^\delta \in \mathcal{R}(A)$, there exists $\mathbf{y} \in \mathbb{R}^d$ such that $\mathbf{b}^\delta = A\mathbf{y}$ thus

$$\begin{aligned} AA^{(\dagger)}\mathbf{b}^\delta &= AA^{(\dagger)}A\mathbf{y} \\ &= U\Sigma Y^t Y^{-t}\Sigma^\dagger U^t U\Sigma Y^t\mathbf{y} \\ &= U\Sigma\Sigma^\dagger\Sigma Y^t\mathbf{y} \\ &= U\Sigma Y^t\mathbf{y} = A\mathbf{y} = \mathbf{b}^\delta, \end{aligned}$$

which concludes the proof. □

Remark 4
We note that $\mathbf{x}_\infty = A^{(\dagger)}\mathbf{b}^\delta$ might not be the minimum norm solution of the system (1), because $\mathbf{x}_\infty$ may have a component in $\mathcal{N}(A)$.

Theorem 3 shows that the iterates determined by Algorithm 1 converge to a solution of (1), when A is a square matrix, for any fixed regularization parameter $\alpha > 0$. This result is useful when the vector $\mathbf{b}^\delta$ is error-free, i.e., when $\delta = 0$ in (2). However, as already mentioned in Section 1 and at the beginning of this subsection, when $\mathbf{b}^\delta$ is error-contaminated, the minimum norm solution $A^\dagger\mathbf{b}^\delta$ typically is severely contaminated by propagated error stemming from the error $\mathbf{e}$ in $\mathbf{b}^\delta$ and, therefore, is not useful. Moreover, the solution $A^{(\dagger)}\mathbf{b}^\delta$ typically is not useful either. A meaningful approximation of $\mathbf{x}^\dagger$ can be determined by terminating the iterations sufficiently early. We will show that the discrepancy principle can be applied to determine when to terminate the iterations. This requires the following auxiliary result.

Lemma 5
Assume that $d = d_1 = d_2 = d_3$ and that (5) holds. Let $\delta > 0$, $\mathbf{b} \in \mathcal{R}(A)$, and $\mathbf{x}_0 = \mathbf{0}$. Then Algorithm 1 terminates after finitely many steps.

Proof
Consider the residual at the limit point

$$\mathbf{r}_k \to \mathbf{r}_\infty = \mathbf{b}^\delta - AA^{(\dagger)}\mathbf{b}^\delta = \left(I - AA^{(\dagger)}\right)(\mathbf{b}+\mathbf{e}) = \left(I - AA^{(\dagger)}\right)\mathbf{e},$$

where in the last step we have used the fact that $\mathbf{b} \in \mathcal{R}(A)$. Now, by (2), we have

$$\|\mathbf{r}_\infty\| = \left\|\left(I - AA^{(\dagger)}\right)\mathbf{e}\right\| \overset{(a)}{\leq} \|\mathbf{e}\| \leq \delta,$$

where the inequality (a) follows from the fact that $I - AA^{(\dagger)}$ in an orthogonal projector; we have

$$I - AA^{(\dagger)} = I - U\Sigma Y^t Y^{-t}\Sigma^\dagger U^t = U(I - \Sigma\Sigma^\dagger)U^t,$$

where U is an orthogonal matrix.

Let $\tau > 1$ be a constant independent of δ. Then there is a constant $k_\tau < \infty$ such that for all $k > k_\tau$, it holds

$$\|\mathbf{r}_k\| < \tau\delta.$$

□

We are now able to prove the regularization property of Algorithm 1.

Theorem 6 (Regularization)
Let $\mathbf{b} \in \mathcal{R}(A)$. Then, under the assumptions of Theorem 3 and Lemma 5, Algorithm 1 terminates as soon as a residual vector $\mathbf{r}_k = \mathbf{b}^\delta - A\mathbf{x}_k$ satisfies $\|\mathbf{r}_k\| \leq \tau\delta$. This stopping criterion is satisfied after finitely many steps $k = k_\delta$. Denote the iterate $\mathbf{x}_{k_\delta}$ simply by $\mathbf{x}^\delta$. Then

$$\limsup_{\delta \searrow 0} \left\|\mathbf{x}^{(\dagger)} - \mathbf{x}^\delta\right\| = 0,$$

where $\mathbf{x}^{(\dagger)} = A^{(\dagger)}\mathbf{b}$.

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Proof
It follows from Lemma 5 that if $\delta > 0$, then the iterations with Algorithm 1 are terminated after finitely many, k, steps. Since $\mathbf{x}_0 = \mathbf{0}$, the iterates determined by the algorithm can be expressed as

$$\mathbf{x}_k = \sum_{j=0}^{k-1} \mathbf{h}_j,$$

where

$$\mathbf{h}_j = A_{\mathcal{N}(L)}^{-1}\mathbf{r}_j + \bar{L}(C^tC + \alpha I)^{-1}C^t\mathbf{r}_j.$$

We first show that

$$A^{(\dagger)}A\mathbf{x}^\delta = \mathbf{x}^\delta.$$

Consider

$$\begin{aligned}
A^{(\dagger)}A\mathbf{h}_j &= A^{(\dagger)}A(A_{\mathcal{N}(L)}^{-1} + \bar{L}(C^tC + \alpha I)^{-1}C^t)\mathbf{r}_j \\
&= Y^{-t}\Sigma^\dagger\Sigma Y^t(Y^{-t}\Sigma^\dagger(I - \Lambda^\dagger\Lambda)U^t + Y^{-t}\Lambda^\dagger(\Gamma^2 + \alpha I)^{-1}\Gamma^t U^t)\mathbf{r}_j \\
&= (Y^{-t}\Sigma^\dagger\Sigma\Sigma^\dagger(I - \Lambda^\dagger\Lambda)U^t + Y^{-t}\Sigma^\dagger\Sigma\Lambda^\dagger(\Gamma^2 + \alpha I)^{-1}\Gamma^t U^t)\mathbf{r}_j \\
&= (Y^{-t}\Sigma^\dagger(I - \Lambda^\dagger\Lambda)U^t + Y^{-t}\Lambda^\dagger(\Gamma^2 + \alpha I)^{-1}\Gamma^t U^t)\mathbf{r}_j = \mathbf{h}_j.
\end{aligned}$$

Thus, we obtain

$$A^{(\dagger)}A\mathbf{x}^\delta = \sum_{j=0}^{k_\delta - 1} A^{(\dagger)}A\mathbf{h}_j = \sum_{j=0}^{k_\delta - 1} \mathbf{h}_j = \mathbf{x}^\delta.$$

Therefore,

$$\begin{aligned}
\limsup_{\delta\searrow 0} \left\|\mathbf{x}^{(\dagger)} - \mathbf{x}^\delta\right\| &= \limsup_{\delta\searrow 0} \left\|A^{(\dagger)}A\left(\mathbf{x}^{(\dagger)} - \mathbf{x}^\delta\right)\right\| \\
&\leq \left\|A^{(\dagger)}\right\| \limsup_{\delta\searrow 0} \left\|A\left(\mathbf{x}^{(\dagger)} - \mathbf{x}^\delta\right)\right\| \\
&= \left\|A^{(\dagger)}\right\| \limsup_{\delta\searrow 0} \left\|\left(\mathbf{b} - \mathbf{b}^\delta\right) + \left(\mathbf{b}^\delta - A\mathbf{x}^\delta\right)\right\| \\
&\leq \left\|A^{(\dagger)}\right\| \limsup_{\delta\searrow 0} (1 + \tau)\,\delta = 0,
\end{aligned}$$

where in the last step we have used the fact that $\mathbf{x}^\delta$ is determined by the discrepancy principle. $\square$

Remark 7
As already mentioned, $A^{(\dagger)}\mathbf{b}$ might not be a minimum norm solution with respect to the Euclidean vector norm. Instead, it is a minimum norm solution with respect to a vector norm induced by the matrix Y^{-t}. We have

$$\left\|A^{(\dagger)}\mathbf{b}\right\| = \left\|Y^{-t}\Sigma U^t\mathbf{b}\right\| = \left\|\Sigma U^t\mathbf{b}\right\|_{Y^{-t}},$$

where we define the norm induced by an invertible matrix $M \in \mathbb{R}^{d\times d}$ as $\|\mathbf{y}\|_M = \|M\mathbf{y}\|$; see, e.g., [14, eq. (5.2.6)]. The norm in the right-hand side is determined by Y^{-t}, which, in turn, is defined by the GSVD (10) of the matrix pair $\{A, L\}$.

3.2. Extension of the convergence analysis to rectangular matrices A and L

We show how the analysis of the previous subsection for square matrices A and L can be extended to rectangular matrices. First consider the case when $A \in \mathbb{R}^{d_1\times d_2}$ with $d_1 < d_2$. We then pad A and $\mathbf{b}^\delta$ with $d_2 - d_1$ zero rows to obtain

$$\widehat{A} = \begin{bmatrix} A \\ O \end{bmatrix} \in \mathbb{R}^{d_2\times d_2}, \qquad \widehat{\mathbf{b}}^\delta = \begin{bmatrix} \mathbf{b}^\delta \\ \mathbf{0} \end{bmatrix} \in \mathbb{R}^{d_2},$$

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and replace A and $\mathbf{b}^\delta$ in (1) by $\widehat{A}$ and $\widehat{\mathbf{b}}^\delta$, respectively. This replacement does not change the solution of the minimization problem (1).

The situation when $A \in \mathbb{R}^{d_1 \times d_2}$ with $d_1 > d_2$ can be handled by padding A with $d_1 - d_2$ zero columns and the solution $\mathbf{x}$ with $d_1 - d_2$ zero rows. We obtain

$$\widehat{A} = [A\ 0] \in \mathbb{R}^{d_1 \times d_1}, \qquad \widehat{\mathbf{x}} = \begin{bmatrix} \mathbf{x} \\ \mathbf{0} \end{bmatrix} \in \mathbb{R}^{d_1},$$

and replace A and $\mathbf{x}$ in (1) by $\widehat{A}$ and $\widehat{\mathbf{x}}$. Only the d_2 first entries of the computed solution are of interest.

The case when $L \in \mathbb{R}^{d_3 \times d_2}$ with $d_3 < d_2$ can be treated similarly as when A has fewer rows than columns. Thus, we pad L with $d_2 - d_3$ zero rows to obtain

$$\widehat{L} = \begin{bmatrix} L \\ O \end{bmatrix} \in \mathbb{R}^{d_2 \times d_2},$$

and replace L in (4) by $\widehat{L}$. This replacement does not affect the computed solution.

Finally, when $L \in \mathbb{R}^{d_3 \times d_2}$ with $d_3 > d_2$, we compute the QR factorization

$$L = QR,$$

where $Q \in \mathbb{R}^{d_3 \times d_2}$ has orthonormal columns and $R \in \mathbb{R}^{d_2 \times d_2}$ is upper triangular. We then replace L in (4) by R. The computed solution is not affected by this replacement.

3.3. *The non-stationary iterated Tikhonov method with a general L*

This section extends the analysis of the stationary iterated Tikhonov regularization method described in Subsection 3.1 and implemented by Algorithm 1 to non-stationary iterated Tikhonov regularization. This extension can be carried out in a fairly straightforward manner. We therefore only state the results and give sketches of proofs.

Consider the iterations

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \left(A^t A + \alpha_k L^t L\right)^{-1} A^t \mathbf{r}_k, \quad k = 0, 1, \dots ,$$

where as usual $\mathbf{r}_k$ denotes the residual vector. We assume that (5) holds and that the regularization parameters $\alpha_k > 0$ satisfy

$$\sum_{k=0}^{\infty} \alpha_k^{-1} = \infty. \tag{22}$$

Analyses of this iteration method when $L = I$ are presented in [7, 8]. The following algorithm outlines the computations with the discrepancy principle as stopping criterion.

Algorithm 2 (GIT$_{NS}$)
Let $A \in \mathbb{R}^{d_1 \times d_2}$, $\mathbf{b}^\delta \in \mathbb{R}^{d_1}$, and $\mathbf{x} \in \mathbb{R}^{d_2}$. Assume that the regularization matrix $L \in \mathbb{R}^{d_3 \times d_2}$ satisfies (5) and that the regularization parameters $\alpha_k > 0$ satisfy (22). Let δ be defined in (2) and fix $\tau > 1$ independently of δ. Let $\mathbf{x}_0 \in \mathbb{R}^{d_2}$ be an available initial approximation of $\mathbf{x}^\dagger$. Compute

for $k = 0, 1, \dots$
  $\mathbf{r}_k = \mathbf{b}^\delta - A\mathbf{x}_k$
  if $\|\mathbf{r}_k\| < \tau\delta$ exit
  $\mathbf{x}_{k+1} = \mathbf{x}_k + \left(A^t A + \alpha_k L^t L\right)^{-1} A^t \mathbf{r}_k$
end.

We would like to show that, under the assumption (22), the iterates determined by the above algorithm without the stopping criterion converge to $A^{(\dagger)}\mathbf{b}^\delta$, and that the algorithm with stopping criterion defines a regularization method. In the remainder of this section, we only consider square matrices A and L. Extensions to rectangular matrices follow as described in Subsection 3.2.

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Theorem 8 (Convergence)
Assume that $d_1 = d_2 = d_3$ and that (5) holds. Let the regularization parameters $\alpha_k > 0$ satisfy (22). Then the iterates determined by Algorithm 2 without stopping criterion converge to the solution $A^{(\dagger)}\mathbf{b}^\delta$ of the linear system of equations $A\mathbf{x} = \mathbf{b}^\delta$.

Proof
The result can be shown in a similar fashion as Theorem 3. We therefore only outline the proof. Similarly as in the proof of Propositions 1 and 2, we split the iterates as

$$\mathbf{x}_k = \mathbf{x}_k^{(0)} + \mathbf{x}_k^{\perp}.$$

Using the GSVD (10) we can show that

$$\mathbf{x}_k^{(0)} \to A_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta \text{ as } k \to \infty, \tag{23}$$
$$\mathbf{x}_k^{\perp} \to \bar{L}C^\dagger\bar{\mathbf{b}}^\delta \text{ as } k \to \infty. \tag{24}$$

Similarly as in Proposition 1, one can show that $\mathbf{x}_k^{(0)} = A_{\mathcal{N}(L)}^{-1}\mathbf{b}^\delta$ for all k. For the $\mathbf{x}_k^{\perp}$ it holds that

$$\mathbf{x}_{k+1}^{\perp} = \bar{L}\tilde{\mathbf{x}}_{k+1} = \sum_{i=0}^{k}(C^tC + \alpha_i I)^{-1}C^t(\bar{\mathbf{b}}^\delta - C\tilde{\mathbf{x}}_i).$$

Using the assumption (22) and [7, Theorem 1.4], it follows that

$$\tilde{\mathbf{x}}_k \to C^\dagger\bar{\mathbf{b}}^\delta \text{ as } k \to \infty.$$

By continuity of $\bar{L}$, we obtain

$$\mathbf{x}_k^{\perp} \to \bar{L}C^\dagger\bar{\mathbf{b}}^\delta \text{ as } k \to \infty.$$

Combining (23) and (24) shows the theorem. □

The following result follows similarly as Theorem 6. We therefore omit the proof.

Theorem 9 (Regularization)
Let the assumptions of Theorem 8 and Lemma 5 hold. Then Algorithm 2 (with stopping crierion) terminates when a residual vector $\mathbf{r}_k = \mathbf{b}^\delta - A\mathbf{x}_k$ satisfies $\|\mathbf{r}_k\| \leq \tau\delta$. This stopping criterion is satisfied after finitely many steps $k = k_\delta$. Denote the iterate $\mathbf{x}_{k_\delta}$ simply by $\mathbf{x}^\delta$. Then

$$\limsup_{\delta\searrow 0}\left\|\mathbf{x}^{(\dagger)} - \mathbf{x}^\delta\right\| = 0.$$

4. NUMERICAL EXAMPLES

This section presents some computed examples where we illustrate the performances of both the stationary and non-stationary iterated Tikhonov methods with general penalty term, referred to as GIT and GIT$_{NS}$, respectively. We first consider three test problems in one space-dimension. These problems are from Regularization Tools by Hansen [15]. Subsequently an image restoration example in two space-dimensions is considered.

The $d_2 \times d_2$ bidiagonal and tridiagonal matrices

$$L_1 = \begin{pmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \\ & & & 0 \end{pmatrix}, \qquad L_2 = \begin{pmatrix} 0 & 0 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & 0 & 0 \end{pmatrix}.$$

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are scaled discretizations of the first and second derivative operators at equidistant points in one space-dimension. Their null spaces are

$$\mathcal{N}(L_1) = \mathsf{span}\left\{\begin{pmatrix}1\\1\\\vdots\\1\end{pmatrix}\right\}, \qquad \mathcal{N}(L_2) = \mathsf{span}\left\{\begin{pmatrix}1\\1\\\vdots\\1\end{pmatrix}, \begin{pmatrix}1\\2\\\vdots\\d_2\end{pmatrix}\right\}.$$

The matrix L_1 preserves sampling of constant functions, while L_2 also preserves uniform sampling of linear functions; see [3].

We apply the GIT$_{NS}$ algorithm using the geometric sequence of regularization parameters (8). They satisfy

$$\sum_{k=0}^{\infty} \alpha_k^{-1} = \frac{1}{\alpha_0} \sum_{k=0}^{\infty} \frac{1}{q^k} = \infty,$$

which shows that the hypothesis on the regularization parameters of Theorems 8 and 9 hold. We fix $q = 0.8$, while the choice of α_0 will depend on L. The relative reconstruction error of the computed solution $\mathbf{x}_k$ is measured by

$$RRE(\mathbf{x}_k) = \frac{\|\mathbf{x}_k - \mathbf{x}^\dagger\|}{\|\mathbf{x}^\dagger\|}.$$

We compare the GIT and GIT$_{NS}$ methods to classical iterated Tikhonov methods with stationary and non-stationary sequences of regularization parameters, referred to as IT and IT$_{NS}$, respectively. We recall that IT and IT$_{NS}$ can be obtained as special cases of GIT and GIT$_{NS}$, respectively, by choosing $L = I$. All problems in one space-dimension have square matrices $A \in \mathbb{R}^{1000\times 1000}$. The matrices A and error-free vectors $\mathbf{b}$ are determined by MATLAB functions in [15]. We define the error-contaminated vector $\mathbf{b}^\delta$ by adding white Gaussian noise to $\mathbf{b}$ with a user-chosen noise level ν such that

$$\nu = \frac{\delta}{\|\mathbf{b}\|}.$$

The iterations with all methods in our comparison are terminated with the discrepancy principle, i.e., we stop the iterations as soon as $\|\mathbf{r}_k\| < \tau\delta$ with $\tau = 1.01$.

As stated in Remark 7, the computed solution may have a component in $\mathcal{N}(A)$. The size of this component depends on the matrix Y in (10). We will tabulate the norm of this component for the examples in one space-dimension. The orthogonal projector $P_{\mathcal{N}(A)}$ onto $\mathcal{N}(A)$ is computed with the aid of the SVD of A. We set all singular values smaller than machine epsilon to zero and compute

$$\frac{\|P_{\mathcal{N}(A)}\mathbf{x}^\delta\|}{\|\mathbf{x}^\delta\|},$$

for the non-stationary algorithms for both the IT and GIT.

Baart We consider the example `baart` and fix $\nu = 0.01$. Figure 2(a) shows the desired solution $\mathbf{x}^\dagger$, a uniform sampling of $\sin(t)$ with $t \in [0, \pi]$, and the right-hand side $\mathbf{b}^\delta$. Consider first stationary iterated Tikhonov. Figure 1(a) shows the RRE for computed solutions determined by the discrepancy principle for $L = I$, $L = L_1$, and $L = L_2$. The regularization parameter $\alpha > 0$ has to be chosen differently for the different regularization matrices. For instance, α has to be chosen much larger for $L = L_2$ than for $L = I$. This is due to the fact that $\mathbf{x}^\dagger$ has a large component in $\mathcal{N}(L_2)$. Therefore, α has to be fairly large to make the penalty term $\alpha\|L_2\mathbf{x}\|^2$ effective. We remark that Algorithm 1 converges for any $\alpha > 0$, but the rate of convergence is affected by the choice of α. Choosing α in a proper range, we observe a substantial reduction of the RRE when using GIT with L_1 and, in particular with L_2, when compared with $L = I$. We set the maximum number of iterations to 10^4. Large values of α did not result in accurate approximations of $\mathbf{x}^\dagger$ within this number of iterations.

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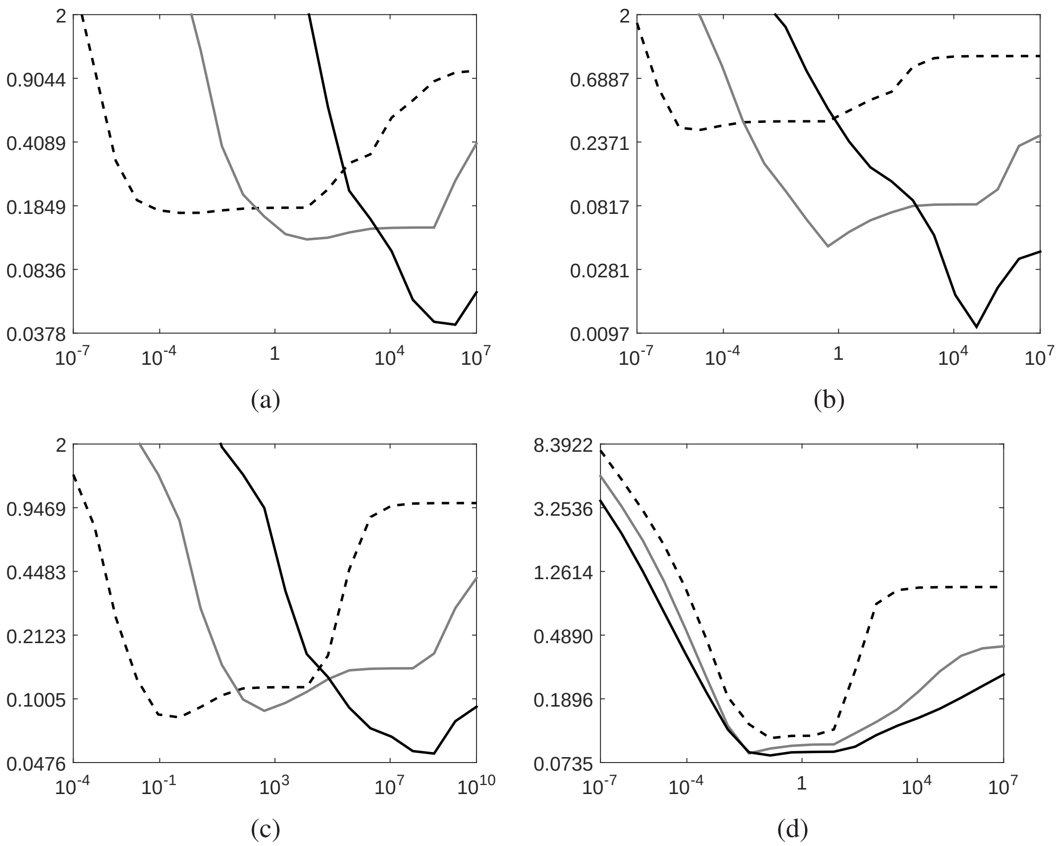

Figure 1. Stationary iterated Tikhonov regularization: RRE for the iterate determined by the discrepancy principle for different values of α: (a) Baart test problem, (b) Deriv2 test problem, (c) Gravity test problem, (d) Peppers test problem. The dashed curves are for $L = I$, the solid gray curves for $L = L_1$, and the solid black curves for $L = L_2$.

For the sake of completeness, we show the number of iterations needed for each tested value of α in Figure 3(a). We see that the number of iterations needed to satisfy the discrepancy principle increases with α. For α sufficiently large, Algorithm 1 terminates because the maximum number of iterations, 10^4, has been reached. For the regularization matrix L_2, a large value of α is required for the regularization term $\alpha \left\| L\mathbf{x} \right\|^2$ to be effective (see Figure 1(a)). Therefore, the tested α-values are not large enough to show a significant increase in the number of iterations.

We would like to mention that the qualitative behavior of the curves in Figure 1 does not depend on the noise level. For instance, consider the `baart` example with noise level $\nu = 0.05$ and apply the GIT algorithm with $L \in \{I, L_1, L_2\}$ for α-values in the range $[10^{-7}, 10^7]$. Figure 3(b) displays the RRE in the approximate solutions determined by Algorithm 1 for the α-values. Comparing Figures 1(a) and 3(b) shows the errors in the computed approximate solutions to differ for $\nu = 0.01$ and $\nu = 0.05$; the computed approximate solutions determined for $\nu = 0.01$ are more accurate. However, the qualitative behavior of the curves is similar.

In the following examples we will not show plots analogous to those of Figure 3, because they are quite similar.

We turn to non-stationary iterations. Comparing the RREs in Table I, we can see that both $L = L_1$ and $L = L_2$ yield more accurate approximations of $\mathbf{x}^\dagger$ than $L = I$. This is also confirmed by visual inspection of the computed solutions in Figure 2(b). Table I shows that the components of the computed solutions in $\mathcal{N}(A)$ are small for the GIT$_{NS}$ methods. Their size depends on the matrix L. This is to be expected since the presence of a component $\mathcal{N}(A)$ is due to L. We obtain a much

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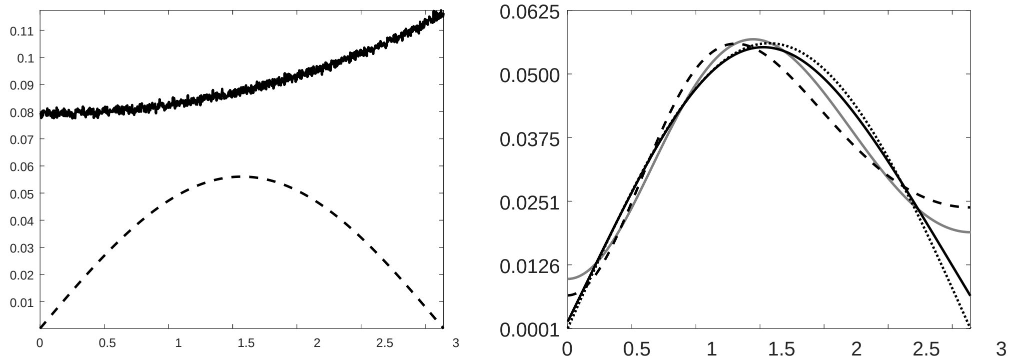
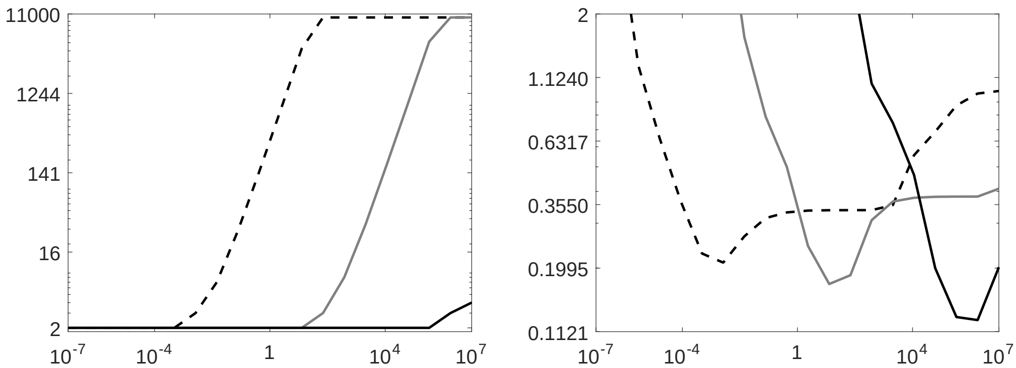


(a) (b)

Figure 2. Baart test problem: (a) desired solution $\mathbf{x}^\dagger$ (dashed curve) and error-contaminated data vector $\mathbf{b}^\delta$ (solid curve), (b) Reconstructions obtained with the non-stationary iterated Tikhonov method with $L = I$ (dashed curve), with $L = L_1$ (solid gray curve), and with $L = L_2$ (solid black curve). The dotted curve shows the desired solution $\mathbf{x}^\dagger$.



(a) (b)

Figure 3. Baart test problem: (a) Number of iterations prescribed by the discrepancy principle using GIT with $\nu = 0.01$ as a function of α, (b) RRE for the iterates determined by the discrepancy principle using GIT with $\nu = 0.05$ for different values of α. The dashed curves are for $L = I$, the solid gray curves for $L = L_1$, and the solid black curves for $L = L_2$.

smaller component in $\mathcal{N}(A)$ for L_1 than for L_2. Nevertheless, the latter regularization matrix gives a more accurate approximation of $\mathbf{x}^\dagger$.

We remark that the dimension of the numerical null space of A is very large, about 990. This may contribute to the fact that the computed solutions do not have negligible components in $\mathcal{N}(A)$. The matrices A in the following examples in one space-dimension have numerical null spaces of much smaller dimension, and the computed approximate solutions have a much smaller component in $\mathcal{N}(A)$. We finally note that the IT_{NS} method yields a negligible component in $\mathcal{N}(A)$.

Deriv2 We now consider the example `deriv2` with $\nu = 0.05$. Figure 4(a) displays the desired solution $\mathbf{x}^\dagger$ and the data vector $\mathbf{b}^\delta$. The vector $\mathbf{x}^\dagger$ is a uniform sampling of the function e^t with $t \in [0, 1]$.

Figure 1(b) shows results for the stationary iterated Tikhonov method. The results are comparable to those of the previous example, but the range of α-values that yield reasonably fast convergence is smaller. A proper estimation of α can be avoided by using non-stationary iterated Tikhonov methods. For the latter methods $L = L_1$ and $L = L_2$ yield approximate solutions of higher quality

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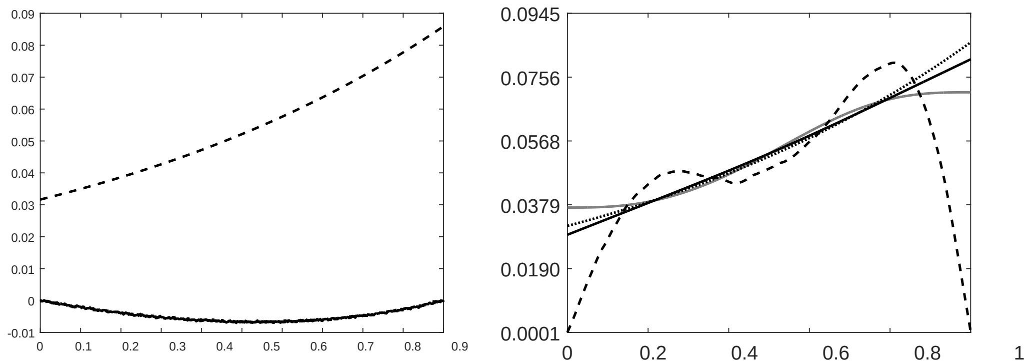
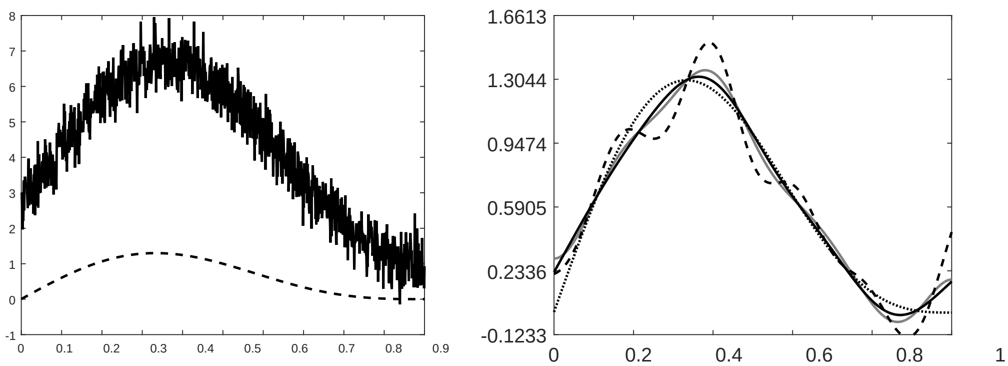
Method	α_0	RRE	Iterations	$\frac{\|P_{\mathcal{N}(A)}\mathbf{x}^\delta\|}{\|\mathbf{x}^\delta\|}$
IT$_{NS}$	10^{-2}	0.17131	4	1.7815×10^{-15}
GIT$_{NS}$ L_1	10^2	0.12331	3	9.1999×10^{-15}
GIT$_{NS}$ L_2	10^6	0.04290	2	0.0027300

Table I. Baart test problem: RRE, number of iterations, and relative magnitude of $P_{\mathcal{N}(A)}\mathbf{x}^\delta$ for the non-stationary iterated Tikhonov method with $L = I$ (IT$_{NS}$), and with $L = L_1$ and L_2 (GIT$_{NS}$). The sequence of α_k is defined by (8) with α_0 shown in the table and $q = 0.8$ for all methods.



(a) (b)

Figure 4. Deriv2 test problem: (a) desired solution $\mathbf{x}^\dagger$ (dashed curve) and error-contaminated data vector $\mathbf{b}^\delta$ (solid curve), (b) Reconstructions obtained with the non-stationary iterated Tikhonov method with $L = I$ (dashed curve), with $L = L_1$ (solid gray curve), and with $L = L_2$ (solid black curve). The dotted curve shows the desired solution $\mathbf{x}^\dagger$.



(a) (b)

Figure 5. Gravity test problem: (a) desired solution $\mathbf{x}^\dagger$ (dashed curve) and error-contaminated data vector $\mathbf{b}^\delta$ (solid curve), (b) Reconstructions obtained with the non-stationary iterated Tikhonov method with $L = I$ (dashed curve), with $L = L_1$ (solid gray curve), and with $L = L_2$ (solid black curve). The dotted curve shows the desired solution $\mathbf{x}^\dagger$.

than $L = I$; see Table II as well as Figure 4(b). The regularization matrix L_2 gives the best result. Table II shows that for all methods the computed approximate solutions have a negligible component in $\mathcal{N}(A)$.

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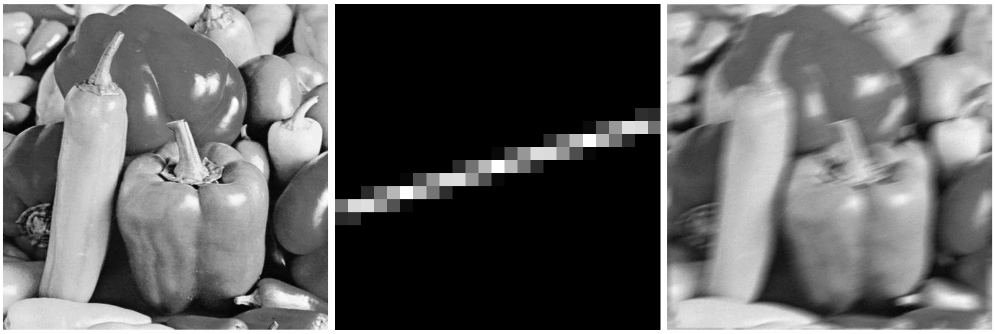
Method	α_0	RRE	Iterations	$\frac{\|P_{\mathcal{N}(A)}\mathbf{x}^\delta\|}{\|\mathbf{x}^\delta\|}$
IT_{NS}	10^{-2}	0.32502	18	2.9408×10^{-15}
$\text{GIT}_{NS}\ L_1$	10^{2}	0.07138	5	2.8801×10^{-15}
$\text{GIT}_{NS}\ L_2$	10^{6}	0.02748	2	2.8411×10^{-15}

Table II. Deriv2 test problem: RRE, number of iterations, and relative magnitude of $P_{\mathcal{N}(A)}\mathbf{x}^\delta$ for the non-stationary iterated Tikhonov method with $L = I$ (IT_{NS}), and with $L = L_1$ and L_2 (GIT_{NS}). The sequence of α_k is defined by (8) with α_0 shown in the table and $q = 0.8$ for all methods.



(a) (b) (c)

Figure 6. Peppers test problem: (a) Uncontaminated image (512×512 pixels), (b) PSF (25×25 pixels), (c) blur- and noise-contaminated image ($\|\mathbf{e}\| = 0.03\,\|\mathbf{b}\|$).

Method	α_0	RRE	Iterations	$\frac{\|P_{\mathcal{N}(A)}\mathbf{x}^\delta\|}{\|\mathbf{x}^\delta\|}$
IT_{NS}	10^{-2}	0.17001	2	4.1708×10^{-15}
$\text{GIT}_{NS}\ L_1$	10^{2}	0.10165	2	1.4004×10^{-9}
$\text{GIT}_{NS}\ L_2$	10^{6}	0.081483	2	6.4620×10^{-10}

Table III. Gravity test problem: RRE, number of iterations, and relative magnitude of $P_{\mathcal{N}(A)}\mathbf{x}^\delta$ for the non-stationary iterated Tikhonov method with $L = I$ (IT_{NS}), and with $L = L_1$ and L_2 (GIT_{NS}). The sequence of α_k is defined by (8) with α_0 shown in the table and $q = 0.8$ for all methods.

Gravity The last example in one space-dimension is `gravity`. We add white Gaussian noise to the error-free data vector $\mathbf{b}$ to determine an error-contaminated data vector $\mathbf{b}^\delta$ with $\nu = 0.1$. The desired solution, $\mathbf{x}^\dagger$, is a uniform sampling of $\sin(\pi t) + \frac{1}{2}\sin(2\pi t)$ with $t \in [0, 1]$. Both $\mathbf{x}^\dagger$ and $\mathbf{b}^\delta$ are displayed in Figure 5(a).

Figure 1(c) shows the RRE values at termination for different α-values for stationary iterated Tikhonov methods. The graphs are similar to those of the previous examples. Table III compares RREs obtained for non-stationary iterated Tikhonov methods. We observe that all non-stationary methods in our comparison converge in only 2 iterations. This is due to the large amount of noise in $\mathbf{b}^\delta$. The more error in $\mathbf{b}^\delta$, the faster the discrepancy principle is satisfied. Similarly as in the previous examples, we see that the use of a regularization matrix different from the identity is beneficial; see Figure 5(b). In particular, the approximations of $\mathbf{x}^\dagger$ obtained with GIT_{NS} are smooth despite the high noise level. Looking at the component of the solution in $\mathcal{N}(A)$, we can see that is very small.

Peppers Our last example illustrates the application of Algorithm 2 to an image deblurring problem. The peppers image in Figure 6(a) represents the blur- and noise-free image (the exact image) that is assumed not to be known. We would like to determine an approximation of this image from an available blur- and noise-contaminated version. The latter is constructed by blurring the exact image by motion blur defined by the point-spread function (PSF) shown in Figure 6(b).

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(a) (b) (c)

Figure 7. Peppers test problem: Restorations determined by the non-stationary iterated Tikhonov method with (a) $L = I$, (b) $L = L_1$, and (c) $L = L_2$.

We add white Gaussian noise such that $\nu = 0.03$ to the blurred image. This gives the blur- and noise-contaminated image that is assumed to be available. The PSF defines the matrix A. We ignore boundary effects and use convolution with periodic boundary conditions to define A. Thus, the matrix A is diagonalized by the Fourier matrix. Therefore the matrix A does not have to be stored; only matrix-vector products with A, using the discrete Fourier transform, have to be evaluated.

We use regularization matrices that are a scaled discretization of periodic divergence L_1 or a scaled discretization of the periodic Laplacian L_2 as follows. Let L_1^1 be defined by

$$L_1^1 = \begin{pmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \\ 1 & & & -1 \end{pmatrix},$$

which is the discretization of the first derivative in one space-dimension with periodic boundary conditions. Then

$$L_1 = L_1^1 \otimes I + I \otimes L_1^1, \tag{25}$$

where I denotes the identity matrix and $\otimes$ the Kronecker product. Similarly, we define

$$L_2 = L_2^1 \otimes I + I \otimes L_2^1, \tag{26}$$

where

$$L_2^1 = \begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix}$$

denotes the discretization of the second derivative in one space-dimension with periodic boundary conditions. Both L_1 and L_2 are BCCB (block circulant with circulant block) matrices and therefore can be diagonalized using the 2D discrete Fourier transform.

We first consider the stationary iterated Tikhonov method. Figure 1(d) displays the RRE of the approximate solution determined by using the discrepancy principle for different values of α. We get stagnation for large α-values. Moreover, for every $\alpha > 0$, the stationary iterated Tikhonov method with L given by (25) or (26) gives better results than with $L = I$ for the same α-value.

Turning to the non-stationary iterated Tikhonov method, Table IV illustrates that the use of the regularization matrices L_1 and L_2 gives smaller errors in the computed approximate solutions than when the identity matrix is used as regularization matrix. Figure 7 shows that the regularization matrices L_1 and L_2 give restorations with less "ringing" and with sharper edges than when using the identity as regularization matrix.

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Method	RRE	Iterations
IT_{NS}	0.10743	7
$\text{GIT}_{NS}\ L_1$	0.09368	4
$\text{GIT}_{NS}\ L_2$	0.08516	3

Table IV. Peppers test problem: RRE and number of iterations for the non-stationary iterated Tikhonov method with $L = I$ (IT_{NS}), and with $L = L_1$ and L_2 (GIT_{NS}). The sequence of α_k is defined by (8) with $\alpha_0 = 1$ and $q = 0.8$ for all methods.

5. CONCLUSIONS

In this paper we have analyzed a generalization of the well-known (stationary) iterated Tikhonov method. This generalization allows the use of an arbitrary regularization matrix L (such that $\mathcal{N}(L) \cap \mathcal{N}(A) = \{0\}$). The numerical results show that the proposed method is robust and that, by choosing an appropriate regularization matrix, it is possible to determine accurate approximate solutions of ill-posed problems. We also introduced a non-stationary version of the algorithm that circumvents the estimation of the Tikhonov regularization parameter. Finally, we want to stress that the method proposed, due to Theorem 3, also can be applied to the solution of well-posed problems.

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