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A modified Tikhonov regularization method☆

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ABSTRACT

Tikhonov regularization and truncated singular value decomposition (TSVD) are two elementary techniques for solving a least squares problem from a linear discrete ill-posed problem. Based on these two techniques, a modified regularization method is proposed, which is applied to an Arnoldi-based hybrid method. Theoretical analysis and numerical examples are presented to illustrate the effectiveness of the method.

1. Introduction

Consider a linear least-squares problem:

$$\min_{x\in\mathbb{R}^n} \|Ax-b\|, \quad A\in\mathbb{R}^{m\times n},\ m\geq n, \tag{1}$$

where and throughout this paper, $\|\cdot\|$ denotes the Euclidean vector norm or the corresponding induced matrix norm. The singular values of the matrix A are assumed of different orders of magnitude close to the origin and some of them may vanish. The minimization problem with a matrix of ill-determined rank is often referred to as a linear discrete ill-posed problem. It may be obtained by discretizing linear ill-posed problems, such as Fredholm integral equations of the first kind with a smooth kernel. This type of integral equations arises in science and engineering when one seeks to determine the cause (the solution) of an observed effect represented by the right-hand side b (the data). Because the entries of b are obtained through observation, they are typically contaminated by a measurement error and also by a discrete error. We denote these errors by $e\in\mathbb{R}^n$ and the unavailable error-free right-hand side associated with b by $\hat{b}\in\mathbb{R}^n$, i.e.,

$$b=\hat{b}+e. \tag{2}$$

We assume that a bound δ for which

$$\|e\|\leq\delta$$

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is available, and the linear system of equations with the unavailable error-free right-hand side

$$Ax = \hat{b} \tag{3}$$

is consistent. Let $\hat{x}$ denote a desired least-squares solution of (3) in the sense of the minimal Euclidean norm. We seek an approximation to $\hat{x}$ by computing an approximate solution of the available linear system of equations (1). Due to the severe ill-conditioning of A and the error e on the right-hand side b, a solution of (1) typically does not yield a meaningful approximation of $\hat{x}$.

The discrete ill-posed problem (1) of small or moderate size is often solved by the truncated singular value decomposition (TSVD) or Tikhonov regularization, see [1,2] for details.

The basis of these two techniques is the singular value decomposition (SVD) defined as

$$A = U\Sigma V^T, \tag{4}$$

where $U = [u_1, u_2, \ldots, u_m] \in \mathbb{R}^{m\times m}$, $U^TU = I$, $V = [v_1, v_2, \ldots, v_n] \in \mathbb{R}^{n\times n}$, $V^TV = I$ and

$$\Sigma = diag[\sigma_1, \sigma_2, \ldots, \sigma_n].$$

Here $(\cdot)^T$ denotes transposition of $(\cdot)$ and the singular values are ordered as

$$\sigma_1 \geq \sigma_2 \geq \sigma_l > \sigma_{l+1} = \cdots = \sigma_n = 0, \quad l = rank(A).$$

The minimum-norm least-squares solution x_{LS} of (1) is

$$x_{LS} = A^+b = \sum_{j=1}^{l} \frac{u_j^Tb}{\sigma_j} v_j,$$

where $A^+ = \sum_{j=1}^{l} v_j\sigma_j^{-1}u_j^T$ is the Moore–Penrose generalized inverse of A.

By ignoring some small singular values, we get the truncated SVD solution x_k given by

$$x_k = A_k^+b = \sum_{j=1}^{k} \frac{u_j^Tb}{\sigma_j} v_j \tag{5}$$

where $k(1 \leq k \leq l)$ is the truncated parameter and $A_k = \sum_{j=1}^{k} u_j\sigma_j v_j^T$.

We note that $x_k \in span\{v_1, v_2, \ldots, v_k\}$. The singular values σ_j and the coefficients u_j^Tb provide a valuable insight about the properties of the linear discrete ill-posed problem (1); see, e.g., [3,2] for a discussion on applications of the TSVD to the linear discrete ill-posed problems.

Instead of solving (1), Tikhonov regularization solves the minimization problem

$$\min_{x\in\mathbb{R}^n}\{\|Ax - b\|^2 + \mu^2\|Lx\|^2\}, \tag{6}$$

which is commonly referred to as a regularization of the problem (1). The scalar $\mu > 0$ is the regularization parameter, and the matrix $L \in \mathbb{R}^{p\times n}(p \leq n)$ is referred to as the regularization matrix, which is chosen either to be the identity matrix I, or a discrete approximation to a derivation operator. The minimization problem (6) is said to be in *standard form* when $L = I$ and in *general form* otherwise. Many examples of regularization matrices can be found in [4–7].

The matrix L is assumed to satisfy

$$N(A) \cap N(L) = \{0\},$$

where $N(\cdot)$ denotes the null space of $(\cdot)$. Then the Tikhonov minimization problem (6) has a unique solution

$$x_\mu = (A^TA + \mu^2L^TL)^{-1}A^Tb; \tag{7}$$

see, e.g., [1,2] for discussions on Tikhonov regularization.

The regularization parameter can be determined in a variety of ways; see, e.g., [8,1,2,9,10]. In our work, we apply the discrepancy principle [1,2,10] to determine the truncation index k and the regularization parameter μ, so that

$$\|Ax_k - b\| \leq \eta\delta, \tag{8}$$

$$\|Ax_\mu - b\| = \eta\delta, \tag{9}$$

where x_k and x_μ are defined in (5) and (7) respectively, and $\eta \geq 1$ is a user-specified constant independent of δ and is usually fairly close to unity.

Thus the truncation index k satisfies

$$\sum_{j=k+1}^{n} (u_j^Tb)^2 \leq (\eta\delta)^2 \leq \sum_{j=k}^{n} (u_j^Tb)^2.$$

Properties of this method are discussed in, e.g., [1,2].

We can use a zero-finder, such as Newton's method, to get the desired value of μ. Further discussion can be found in [1,2,10].

Martin Fuhry in [6] proposed a new method to construct the regularization matrix for Tikhonov regularization that bridges the gap between Tikhonov regularization and TSVD. He introduced

$$L_\mu = D_\mu V^T \tag{10}$$

with

$$D_\mu^2 = diag[\max\{\mu^2 - \sigma_1^2, 0\}, \max\{\mu^2 - \sigma_2^2, 0\}, \ldots, \max\{\mu^2 - \sigma_n^2, 0\}], \tag{11}$$

where μ is the regularization parameter determined by (9). Then the Tikhonov regularization problem (6) can be rewritten as

$$\min_{x\in\mathbb{R}^n}\{\|Ax - b\|^2 + \|L_\mu x\|^2\} \tag{12}$$

with L_μ defined in (10).

By the singular value decomposition, (12) has a solution

$$x_\mu = V(\Sigma^T\Sigma + D_\mu^2)^{-1}\Sigma^T U^T b. \tag{13}$$

For $\sigma_k > \mu \geq \sigma_{k+1}$,

$$\Sigma^T\Sigma + D_\mu^2 = diag[\sigma_1^2, \sigma_2^2, \ldots, \sigma_k^2, \mu^2, \ldots, \mu^2] \in \mathbb{R}^{n\times n}. \tag{14}$$

The matrix (14) is positive definite and the solution (13) is

$$x_\mu = \sum_{j=1}^{l} \varphi_{\mu,j}\frac{u_j^T b}{\sigma_j} v_j, \tag{15}$$

with the filter factors

$$\varphi_{\mu,j} = \begin{cases} 1, & 1 \leq j \leq k, \\ \dfrac{\sigma_j^2}{\mu^2}, & k < j \leq l. \end{cases}$$

Similarly, (1) can be rewritten as

$$x = V(\Sigma^T\Sigma)^{-1}\Sigma^T U^T b,$$

where

$$\Sigma^T\Sigma = diag[\sigma_1^2, \ldots, \sigma_k^2, \ldots, \sigma_n^2]. \tag{16}$$

By comparing (14) and (16), we find that some small singular values $\sigma_i (k+1 \leq i \leq n)$ are replaced by μ. As a consequence, useful information of the exact solution $\hat{x}$ may be lost, which may overdamp the solution components v_j of small index.

In order to get an appropriate solution with improved accuracy, we modify the regularization matrix (10) so as to include more useful information. Theoretical analysis and numerical results show that our method can improve the accuracy of the approximate solutions, almost with the same elapsed CPU time. In Section 3, we apply our modified Tikhonov regularization to an Arnoldi-based hybrid method and a decomposition method discussed in [11].

This paper is organized as follows. In Section 2, our new regularization matrix based on (10) is discussed. In Section 3, we describe the Arnoldi-based hybrid method and review the decomposition method provided in [11]. Numerical examples are presented in Section 4.

2. The modified regularization matrix

In this section, we first describe a modification of the regularization matrix (10), and then show in Section 2.2 how to choose a parameter in the modified regularization matrix.

2.1. The modified regularization matrix

Let us introduce

$$\tilde{L}_\mu = \tilde{D}_\mu V^T, \tag{17}$$

with

$$\tilde{D}_\mu^2 = diag[(1-\omega)\max\{\mu^2 - \sigma_1^2, 0\}, \ldots, (1-\omega)\max\{\mu^2 - \sigma_n^2, 0\}],$$

where the value of μ is the same as that in (11) and the scale $\omega (\omega < 1)$ is a parameter. When $\omega = 0$, $\tilde{D}_\mu$ is equal to D_μ in (11).

Replacing L_μ in (10) by $\tilde{L}_\mu$ we obtain

$$x_\mu = V(\Sigma^T\Sigma + \tilde{D}_\mu^2)^{-1}\Sigma^T U^T b. \tag{18}$$

If $\sigma_k > \mu \geq \sigma_{k+1}$, then

$$\Sigma^T\Sigma + \tilde{D}_\mu^2 = diag[\sigma_1^2, \ldots, \sigma_k^2, (1-\omega)\mu^2 + \omega\sigma_{k+1}^2, \ldots, (1-\omega)\mu^2 + \omega\sigma_n^2],$$

which is a positive definite matrix and (18) is equivalent to

$$x_{\mu,\omega,j} = \sum_{j=1}^{l} \tilde{\varphi}_{\mu,\omega,j}\frac{u_j^T b}{\sigma_j}v_j, \quad \omega < 1, \tag{19}$$

with the filter factors

$$\tilde{\varphi}_{\mu,\omega,j} = \begin{cases} 1, & 1 \leq j \leq k, \\ \dfrac{\sigma_j^2}{(1-\omega)\mu^2 + \omega\sigma_j^2}, & k < j \leq l. \end{cases}$$

Here, for $1 \leq j \leq k$, the filter factors $\tilde{\varphi}_{\mu,\omega,j}$ are the same as $\varphi_{\mu,j}$, while for $k < j \leq l$, the filter factors satisfy

$$\begin{cases} \dfrac{\sigma_j^2}{\mu^2} < \dfrac{\sigma_j^2}{(1-\omega)\mu^2 + \omega\sigma_j^2}, & 0 < \omega < 1 \\ \dfrac{\sigma_j^2}{\mu^2} = \dfrac{\sigma_j^2}{(1-\omega)\mu^2 + \omega\sigma_j^2}, & \omega = 0 \\ \dfrac{\sigma_j^2}{\mu^2} > \dfrac{\sigma_j^2}{(1-\omega)\mu^2 + \omega\sigma_j^2}, & \omega < 0 \end{cases} \Longrightarrow \begin{cases} \tilde{\varphi}_{\mu,\omega,j} < \varphi_{\mu,j}, & 0 < \omega < 1 \\ \tilde{\varphi}_{\mu,\omega,j} = \varphi_{\mu,j}, & \omega = 0 \\ \tilde{\varphi}_{\mu,\omega,j} > \varphi_{\mu,j}, & \omega < 0. \end{cases}$$

The effect of the filter factors is to remove the SVD components corresponding to the smaller singular values, and thereby to stabilize the solution.

Here by adjusting the parameter ω, we could get the optimal filter factor and more useful information. So the solution of (18) may be a better approximation to the desired solution $\hat{x}$ than the solution of (13). The numerical examples in Section 4 will support this inference.

Theorem 2.1.

$$\min_{x\in\mathbb{R}^n}\{\|Ax-b\|^2 + \|\tilde{L}_\mu x\|^2\}$$

is equivalent to

$$\min_{x\in\mathbb{R}^n}\{\|Ax-b\|^2 + (1-\omega)\|L_\mu x\|^2\}, \quad \omega < 1,$$

where $\tilde{L}_\mu$ and L_μ are the regularization matrices in (10) and (17), respectively.

Proof.

$$\begin{aligned} \|\tilde{L}_\mu x\|^2 &= \|\tilde{D}_\mu V^T\|^2 = (\tilde{D}_\mu V^T)^T(\tilde{D}_\mu V^T) = V\tilde{D}_\mu^T\tilde{D}_\mu V^T \\ &= V\tilde{D}_\mu^2 V^T = (1-\omega)VD_\mu^2 V^T = (1-\omega)\|D_\mu V^T\|^2 \\ &= (1-\omega)\|L_\mu x\|^2, \end{aligned}$$

the second equality in the second line is due to $\tilde{D}_\mu^2 = (1-\omega)D_\mu^2$. □

2.2. Choice of the parameter

In this subsection, we first use the discrepancy principle to determine the parameter ω so that $x_{\mu,\omega,j}$ satisfies the discrepancy principle. Introduce the function

$$\phi(\omega) = \|b - Ax_{\mu,\omega,j}\|^2. \tag{20}$$

Then (9) can be expressed as

$$\phi(\omega) = \eta^2\delta^2. \tag{21}$$

Theorem 2.2. *Assume $x_{\mu,\omega,j}$ satisfies (19). Then the function (20) can be expressed as*

$$\phi(\omega) = \sum_{j=k+1}^{l}\left[1 - \frac{\sigma_j^2}{(1-\omega)\mu^2 + \omega\sigma_j^2}\right]^2 (u_j^T b)^2 + \sum_{j=n+1}^{m}(u_j^T b)^2. \tag{22}$$

Consequently, as a function of ω, $\phi(\omega)$ is strictly decreasing and (21) has a unique solution $\tilde{\omega}$ in $(-\infty, 1)$, provided that

$$\sum_{j=n+1}^{m} (u_j^T b)^2 < (\eta\delta)^2 < \sum_{j=k+1}^{l} (u_j^T b)^2 + \sum_{j=n+1}^{m} (u_j^T b)^2. \tag{23}$$

Proof. The formula (22) follows from (19). Thus

$$\frac{\partial}{\partial\omega}\phi(\omega) = \sum_{j=k+1}^{l} \frac{2(\omega-1)(\mu^2-\sigma_j^2)^2\sigma_j^2}{[\mu^2+\omega(\sigma_j^2-\mu^2)]^3}(u_j^T b)^2.$$

Clearly, ϕ is a monotonically decreasing function. Moreover, we obtain from (22) that

$$\lim_{\omega\to 1}\phi(\omega) = \sum_{j=n+1}^{m}(u_j^T b)^2,$$

$$\lim_{\omega\to-\infty}\phi(\omega) = \sum_{j=k+1}^{l}(u_j^T b)^2 + \sum_{j=n+1}^{m}(u_j^T b)^2.$$

Since the function ϕ is decreasing, the upper and the lower bound of (23) have to be satisfied in order for (21) to have a solution in $(-\infty, 1)$. □

Theorem 2.2 shows that the parameter ω can be determined by the discrepancy principle, but the function ϕ is not convex, so the desired value of ω cannot be computed inexpensively by using a zero-finder, such as Newton's method.

In this paper we use generalized cross validation (GCV) [1,2,12] to determine the parameter ω. Denote

$$A^\sharp = V(\Sigma^T\Sigma + \tilde{D}_\mu^2)^{-1}\Sigma^T U^T. \tag{24}$$

Then in (19), $x_{\mu,\omega,j} = A^\sharp b$.

According to the basic idea of GCV, ω can be determined by minimizing GCV function

$$G(\omega) = \frac{\|(I_m - AA^\sharp)b\|_2^2}{(trace(I_m - AA^\sharp))^2} \tag{25}$$

in the range $(-\infty, 1)$.

In order to get the specific form of (25), we first determine a suitable value of the regularization parameter μ such that the associated solution x_μ in (7) with $L = I$ satisfies the discrepancy principle. By Proposition 2.1 in [10], the function $\psi(\mu) = \|Ax_\mu - b\|^2 - \eta^2\delta^2$ can be written as follows:

$$\psi(\mu) = b^T\left(\frac{1}{\mu^2}AA^T + I\right)^{-2} b - \eta^2\delta^2.$$

By using the SVD (4) of A, we have

$$\begin{aligned}\psi(\mu) &= b^T\left(\frac{1}{\mu^2}U\Sigma\Sigma^T U^T + I\right)^{-2} b - \eta^2\delta^2\\ &= \sum_{i=1}^{n}\frac{\tilde{b}_i^2}{\left(\frac{1}{\mu^2}\sigma_i^2+1\right)^2} - \eta^2\delta^2,\end{aligned} \tag{26}$$

where $\tilde{b} = [\tilde{b}_1, \tilde{b}_2, \ldots, \tilde{b}_n]^T = U^T b$.

To get the regularization parameter μ, Newton's method is used to solve $\psi(\mu) = 0$ with initial approximation $\mu_0 = 0$. Then we can determine the parameter k such that $\sigma_k > \mu \geq \sigma_{k+1}$.

Then by (24) and the SVD of A, the numerator of (25) can be written as

$$\|(I_m - AA^\sharp)b\|_2^2 = \sum_{i=k+1}^{n}\left[\frac{\mu^2-\sigma_i^2}{(1-\omega)\mu^2+\omega\sigma_i^2}u_i^T b\right]^2, \tag{27}$$

while the denominator of (25) satisfies

$$(trace(I_m - AA^\sharp))^2 = \left[\sum_{i=k+1}^{n}\frac{\mu^2-\sigma_i^2}{(1-\omega)\mu^2+\omega\sigma_i^2}\right]^2. \tag{28}$$

Combining (27) and (28), we obtain

Theorem 2.3. *If we use GCV to determine the parameter ω, then the GCV function is*

$$G(\omega) = \frac{\sum_{i=k+1}^{n} \left[\frac{\mu^2-\sigma_i^2}{(1-\omega)\mu^2+\omega\sigma_i^2} u_i^T b\right]^2}{\left[\sum_{i=k+1}^{n} \frac{\mu^2-\sigma_i^2}{(1-\omega)\mu^2+\omega\sigma_i^2}\right]^2}, \quad \omega < 1. \tag{29}$$

Some optimization methods can be used to get the minimizer of the GCV function. In this paper, we use MATLAB code *fminbnd* to find the parameter ω in the range $(-\infty, 1)$.

The process of determining ω can be summarized in the following algorithm.

Algorithm 2.1 Determining of the parameter ω

1. Compute the SVD (4) of A;
2. Determine the regularization parameter μ by using Newton's method to the equation $\psi(\mu) = \|Ax_\mu - b\|^2 - \eta^2\delta^2 = 0$;
3. Determine the parameter k such that $\sigma_k > \mu \geq \sigma_{k+1}$;
4. Compute the GCV function $G(\omega)$ in (29);
5. Use MATLAB code *fminbnd* to find the minimizer of function $G(\omega)$ in the range $(-\infty, 1)$.

3. Arnoldi-based hybrid method

It is well-known that GMRES *semiconverges* for ill-posed problem (see [13–17]), i.e., the iterates first seem to converge to the true solution vector before they are misled by noisy components in the data and subsequently deteriorate early. The *semiconvergence* behavior of GMRES can be stabilized by using a *hybrid* method (see [14,18]) that combines an Arnoldi process with a direct regularization scheme. In the following, we review the process of the Arnoldi-based *hybrid* method.

The problem (1) can be reduced to a problem of smaller size by applying a few steps, say l, of Arnoldi process with respect to A starting from the initial vector $u_1 = r_0/\|r_0\|$, $r_0 = b - Ax_0$, and x_0 is the initial approximate solution. This yields the decomposition

$$AU_l = U_{l+1}H_l, \tag{30}$$

where $U_{l+1} = [u_1, u_2, \ldots, u_l, u_{l+1}] \in \mathbb{R}^{n\times(l+1)}$ has orthonormal columns, which span the Krylov subspace

$$\mathbb{K}_l(A, b) = span\{b, Ab, \ldots, A^{l-1}b\}. \tag{31}$$

The matrix $U_l \in \mathbb{R}^{n\times l}$ consists of the first l columns of U_{l+1}. We assume that l is sufficiently small so that $H_l \in \mathbb{R}^{(l+1)\times l}$ is an upper Hessenberg matrix with nonvanishing subdiagonal entries; see, e.g., [19] for details.

Substitute $x = U_l y$ into (1), the least squares problem (1) can be approximated by a smaller problem

$$\min_{y\in\mathbb{R}^l} \|H_l y - e_1\|b\| \|,$$

where $e_1 = [1, 0, \ldots, 0]^T$ is the first Cartesian basis vector in $\mathbb{R}^{l+1}$. Thus each iteration of GMRES requires solving a least squares problem involving an upper Hessenberg matrix H_l. Since the original problem is ill-posed, the matrix H_l may become very ill-conditioned. Therefore, a regularization method must be used to compute

$$y = \|b\| \ \| \ H_l^\dagger e_1.$$

The stopping index l for the Arnoldi process can be determined by the discrepancy principle, i.e., the iterations can be terminated as soon as an approximate solution x_j satisfies

$$\|Ax_j - b\| \leq \eta\delta, \tag{32}$$

where $\eta \geq 1$ is a user-specified constant independent of δ; see [15] for a validity of this stopping criterion.

In this paper, we denote three Tikhonov regularization methods with regularization matrices $L_\mu = \mu I$, (10), and (17) as ST, TT and TTw respectively, and we use the three methods to stabilize the GMRES iteration. Such three *hybrid* methods are represented by GMRES + ST, GMRES + TT, and GMRES + TTw respectively.

The following algorithm implements the Arnoldi-based hybrid method.

Algorithm 3.1 Arnoldi-based hybrid method

1. Input: *maxiter*, parameter ω, η and δ, and initial guess x_0,
   METHOD $\in$ {GMRES + ST, GMRES + TT, GMRES + TTw};
2. Compute $r_0 = b - Ax_0$, $\beta = \|r_0\|$, $v_1 = r_0/\beta$;
3. $V = [\,]$; $V = [V, v_1]$; $H = [\,]$;
4. For $i = 1 : maxiter$
5. $\quad k = size(H, 2) + 1$;
6. $\quad v = AV(:, k)$;
7. $\quad h = zeros(k + 1, 1)$;
8. $\quad$ For $j = 1 : k$
9. $\quad\quad h(j, 1) = V(:, j)^T v$;
10. $\quad\quad v = v - h(j, 1)V(:, j)$;
11. $\quad$ End
12. $\quad h(k + 1, 1) = \|v\|$;
13. $\quad v = v/\|v\|$;
14. $\quad V = [V, v]$;
15. $\quad H = [H, h(1 : k, 1); [zeros(1, k - 1), h(k + 1, 1)]]$;
16. $\quad$ If METHOD $=$ GMRES + ST then
17. $\quad\quad$ Compute $y_{\mu,l} = \min \|Hy - e_1\|b\| \|$ by (7);
18. $\quad\quad x = V(:, 1 : i)y_{\mu,l}$;
19. $\quad$ Elseif METHOD $=$ GMRES + TT then
20. $\quad\quad$ Compute $y_{\mu,l} = \min \|Hy - e_1\|b\| \|$ by (13);
21. $\quad\quad x = V(:, 1 : i)y_{\mu,l}$;
22. $\quad$ Else METHOD $=$ GMRES + TTw then
23. $\quad\quad$ Compute $y_{\mu,\omega,l} = \min \|Hy - e_1\|b\| \|$ by (18);
24. $\quad\quad x = V(:, 1 : i)y_{\mu,\omega,l}$;
25. $\quad$ End
26. $\quad$ If $\|b - Ax\| \leftarrow \eta\delta$;
27. $\quad\quad$ break;
28. End
29. End

3.1. Selective regularization by augmentation

For some linear discrete ill-posed problem (1) the null space $N(L)$ is important, because the solution component in $N(L)$ is determined independently of μ and is therefore not damped. We may choose L so that $N(L)$ represents important known features of the desired solution $\hat{x}$. This section describes how $N(L)$ can be incorporated into the solution process by using the decomposition method described in [11], which has been applied in iterative and direct methods for solving ill-posed problems, see [20–22].

Let the matrix $W \in \mathbb{R}^{n\times l}$, $l \ll n$, has orthonormal columns, which span $N(L)$ or represent pertinent features of $\hat{x}$. These features may be jumps, spikes, or just linear increase. Introduce the QR factorization

$$AW = QR,$$

where $Q \in \mathbb{R}^{m\times l}$ is orthonormal in columns and $R \in \mathbb{R}^{l\times l}$ is upper triangular. We assume that W is chosen so that R is nonsingular. Define the orthogonal projectors

$$P_W = WW^T, \qquad P_W^{\perp} = I - WW^T, \qquad P_Q = QQ^T, \qquad P_Q^{\perp} = I - P_Q.$$

Then (1) can be written as

$$\begin{aligned}\min_{x\in\mathbb{R}^n} \|Ax - b\|^2 &= \min_{x\in\mathbb{R}^n} \|P_Q Ax - P_Q b\|^2 + \|P_Q^{\perp} Ax - P_Q^{\perp} b\|^2 \\ &= \min_{x\in\mathbb{R}^n} \|P_Q AP_W x - (P_Q b - P_Q AP_W^{\perp} x)\|^2 + \|P_Q^{\perp} AP_W^{\perp} x - P_Q^{\perp} b\|^2,\end{aligned}$$

where we have used the fact $P_Q^{\perp} AP_W = 0$. It follows that

$$\min_{x\in\mathbb{R}^n} \|P_Q AP_W x - (P_Q b - P_Q AP_W^{\perp} x)\| = \|Ry - Q^T(b - AP_W^{\perp} x)\|, \tag{33}$$

where $y = W^T x$. Because R is nonsingular, we may choose y for any $P_W^{\perp} x$ so that the right-hand side in (33) vanishes. Thus we get

$$\min_{x\in\mathbb{R}^n} \|Ax - b\| = \min_{x\in\mathbb{R}^n} \|P_Q^{\perp} A P_W^{\perp} x - P_Q^{\perp} b\|. \tag{34}$$

The projected problem on the right-hand side is also an ill-posed problem, which can be solved by an iterative regularization method or a direct regularization method. Serena Morigi [13] used TSVD and Baglama J [11] used GMRES-type iterative regularization methods to the projected problems (34). In our work, we apply three direct methods ST, TT and TTw to this problem, and make some comparisons. Denote the computed approximate solution of (33) and (34) by x' and x'' respectively. Thus the corresponding solution of (1) is given by $x = x' + x''$.

4. Numerical experiments

In this section, we first discuss the flop counts for the methods in Sections 2 and 3. Then we give some examples to illustrate the effectiveness of our method.

We consider the computational complexity for the case $m = n$. Note that the main arithmetic work for each of the three Tikhonov regularization methods ST, TT and TTw is the SVD factorization (4) which needs $O(n^3)$ flops, see in [23, p. 254], and the evaluation of every solution of (7), (15) and (19) can be carried out in $O(n^2)$ flops. Each of the three direct methods has the complexity of order of n^3. We assume the number of iteration in Algorithm 3.1 is l. Here and in the sequel, l represents l_{ST}, l_{TT}, and $l_{TT\omega}$ for GMRES + ST, GMRES + TT, and GMRES + TTw respectively. The dominant arithmetic work for each of the three *hybrid* methods is the Gram–Schmidt procedure in the 4th to 13th lines of Algorithm 3.1 which needs $O(nl^2)$ flops, see in [24, p. 165], and the computation for the solution of the smaller problem (32) in the 17th, 20th and 23th lines of Algorithm 3.1, where $O(l^4)$ flops are required. In summary, each of the three *hybrid* methods has the complexity of order $nl^2 + l^4$ which is determined by the iteration number l.

The error-free $\hat{b}$ is available by

$$\hat{b} = A\hat{x}. \tag{35}$$

The error vector e has normally distributed entries with zero mean and is scaled so that the contaminated b, defined by (2), has a specified noise level relative error

$$\epsilon = \|e\|/\|\hat{b}\|. \tag{36}$$

The initial approximate solution $x_0 = 0$ in Algorithm 3.1 is used for all the iterative methods and the parameter η is set to 1 in all examples. The regularization parameter μ and the truncated index k are determined by the discrepancy principle. The parameter ω in (17) is determined by the GCV function.

In this section, we give two kinds of comparison of numerical results. One is among the three Tikhonov regularization methods, the other is among GMRES and the three *hybrid* methods.

The first three examples compare three Tikhonov regularization methods.

Example 4.1. The Fredholm integral equation of the first kind

$$\int_{-6}^{6} K(s,t)x(t)dt = g(s), \quad -6 \le s \le 6, \tag{37}$$

with the kernel and the solution given by

$$k(s,t) := x(s-t),$$
$$x(t) := \begin{cases} 1 + \cos\left(\frac{\pi}{3}t\right), & |t| < 3, \\ 0, & \text{otherwise.} \end{cases}$$

The right-hand side function $g(s)$ is defined by (37). This integral equation is discussed by Phillips [25].

We discretize the integral equation by the Galerkin method with orthonormal box functions as test and trial functions by the MATLAB program *phillips* from Regularization Tools [26] and obtain the matrix $A \in \mathbb{R}^{200\times 200}$ and the discretized solution $\hat{x}$ of the error-free linear system (3). The error-free right-hand side $\hat{b}$ is given by (35). The associated contaminated vector b in (1) is obtained by adding 0.1% normally distributed zero mean "noise" e to $\hat{b}$; cf. (2). Thus, $\epsilon = 1 \cdot 10^{-3}$ in (36).

Table 1 reports the relative errors and the CPU time of Example 4.1. The table shows that the approximate solution computed by TTw is the most accurate, and the elapsed CPU time is almost the same as those of the ST and the TT methods.

Example 4.2. The Fredholm integral equation of the first kind

$$\int_{0}^{1} K(s,t)x(t)dt = g(s), \quad 0 \le s \le 1, \tag{38}$$

Table 1
Relative errors and CPU time of the numerical solutions for Example 4.1.

Tikhonov regularization	Relative error	CPU (s)
ST ($L_\mu = \mu I$)	$1.10 \cdot 10^{-2}$	0.124
TT (L_μ defined by (10))	$1.10 \cdot 10^{-2}$	0.127
TTw (L_μ defined by (17))	$9.70 \cdot 10^{-3}$	0.124

Table 2
Relative errors and CPU time of the numerical solutions for Example 4.2.

Tikhonov regularization	Relative error	CPU (s)
ST ($L_\mu = \mu I$)	$1.61 \cdot 10^{-1}$	0.110
TT (L_μ defined by (10))	$1.52 \cdot 10^{-1}$	0.108
TTw (L_μ defined by (17))	$9.30 \cdot 10^{-2}$	0.111

Table 3
Relative errors and CPU time of the numerical solutions for Example 4.3.

Tikhonov regularization	Relative error	CPU (s)
ST ($L_\mu = \mu I$)	$1.62 \cdot 10^{-1}$	0.021
TT (L_μ defined by (10))	$1.37 \cdot 10^{-1}$	0.022
TTw (L_μ defined by (17))	$5.06 \cdot 10^{-2}$	0.022

with the kernel and the solution given by

$$k(s,t) := d(d^2 + (s-t)^2)^{-3/2}, \quad d = 0.25.$$
$$x(t) := \sin(\pi t) + \frac{1}{2}\sin(2\pi t).$$

The right-hand side function $g(s)$ is defined by (38). This integral equation is discussed by Wing [27].

We discretize the integral equation by the Galerkin method with orthonormal box functions as test and trial functions by the MATLAB code *gravity* from [26] and obtain the matrix $A \in \mathbb{R}^{200\times 200}$ and the discretized solution $\hat{x}$ of the error-free linear system (3). The error-free right-hand side $\hat{b}$ is given by (35). The associated contaminated vector b in (1) is obtained by adding 50% normally distributed zero mean "noise" e to $\hat{b}$; cf. (2). Thus, $\epsilon = 5 \cdot 10^{-1}$ in (36).

Table 2 reports the relative errors and the CPU time of Example 4.2. The table shows that the approximate solution computed by TTw is the most accurate, and the elapsed CPU time is almost the same as those of the ST and the TT methods.

Example 4.3. We consider the equation $Ax = b$.

Let $A \in \mathbb{R}^{100\times 100}$ be a Hilbert matrix computed with the MATLAB program *hilb*(100) and the solution $\hat{x} = [1, 1, \ldots, 1] \in \mathbb{R}^{100}$. The condition number of matrix A is 1.46e + 20. The error-free right-hand side vector $\hat{b}$ is given by (35). The associated contaminated vector b in (1) is obtained by adding 10% normally distributed zero mean "noise" e to $\hat{b}$; cf. (2). Thus, $\epsilon = 1 \cdot 10^{-1}$ in (36).

Table 3 reports the relative errors and the CPU time of Example 4.3. The table shows that the approximate solution computed by TTw is the most accurate, and the elapsed CPU time is almost the same as those of the ST and the TT methods.

The following three examples illustrate the effect of three hybrid methods.

Example 4.4. The Fredholm integral equation of the first kind

$$\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} K(s,t)x(t)dt = g(s), \qquad -\frac{\pi}{2} \le s \le \frac{\pi}{2}, \tag{39}$$

with the kernel and the solution given by

$$k(s,t) := (\cos(s) + \cos(t))\left(\frac{\sin(u)}{u}\right)^2, \quad u = \pi(\sin(s) + \sin(t)).$$
$$x(t) := \sin(t).$$

The right-hand side function $g(s)$ is defined by (39). This integral equation is discussed by Shaw [28].

We discretize the integral equation by the Galerkin method with orthonormal box functions as test and trial functions by the MATLAB program *shaw* from Regularization Tools [26] and obtain the matrix $A \in \mathbb{R}^{2000\times 2000}$ and the discretized solution

Table 4
Arnoldi steps, relative errors and CPU time of the numerical solutions for Example 4.4.

Method		Arnoldi step	Relative error	CPU (s)
GMRES		10	$2.85 \cdot 10^{-1}$	0.295
hybrid method	GMRES + ST	11	$2.16 \cdot 10^{-2}$	0.504
	GMRES + TT	19	$1.01 \cdot 10^{0}$	0.790
	GMRES + TTw	15	$1.99 \cdot 10^{-2}$	0.644

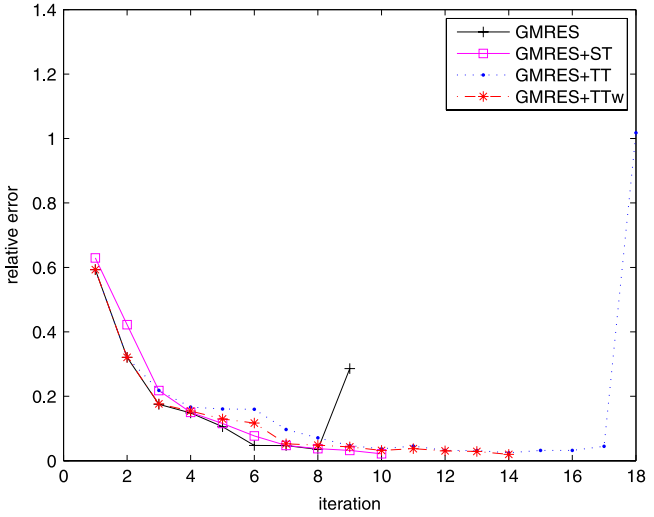

Fig. 1. Example 4.4: Norm of relative errors in iterates generated by GMRES, GMRES + ST, GMRES + TT and GMRES + TTw.

$\hat{x}$ of the error-free linear system (3). The error-free right-hand side $\hat{b}$ is given by (35). The associated contaminated vector b in (1) is obtained by adding 0.001% normally distributed zero mean "noise" e to $\hat{b}$; cf. (2). Thus, $\epsilon = 1 \cdot 10^{-5}$ in (36).

Table 4 reports the Arnoldi steps, the relative errors and the CPU time of Example 4.4. We note that GMRES requires the fewest Arnoldi step and CPU time, while it achieves the larger relative error than GMRES + ST and GMRES + TTw. We also can see that GMRES + TT does not reduce the relative error as much as the other two hybrid methods. Furthermore, GMRES + TTw achieves the slightly smaller relative error than GMRES + ST.

Fig. 1 displays the relative error for iterates x_j determined by the three hybrid methods. This figure shows that both GMRES + ST and GMRES + TTw can stabilize the *semiconvergence* of GMRES.

Example 4.5. The Fredholm integral equation of the first kind

$$\int_0^{\infty} K(s,t)x(t)dt = g(s), \quad s \geq 0, \tag{40}$$

with the kernel and the solution given by

$$k(s,t) := \exp(-st),$$
$$x(t) := \exp(-t/2).$$

The right-hand side function $g(s)$ is defined by (40). This integral equation is discussed by Varah [29].

We discretize the integral equation by the Galerkin method with orthonormal box functions as test and trial functions by the MATLAB program *ilaplace* from Regularization Tools [26] and obtain the matrix $A \in \mathbb{R}^{2000\times 2000}$ and the discretized solution $\hat{x}$ of the error-free linear system (3). The error-free right-hand side $\hat{b}$ is given by (35). The associated contaminated vector b in (1) is obtained by adding 0.1% normally distributed zero mean "noise" e to $\hat{b}$; cf. (2). Thus, $\epsilon = 1 \cdot 10^{-3}$ in (36).

Table 5 reports the Arnoldi steps, the relative errors and the CPU time of Example 4.5. GMRES requires the fewest Arnoldi steps and CPU time, while it achieves the worst relative error. For the three hybrid methods, GMRES + TTw yields the best approximate solution, and the elapsed CPU time is almost the same as those of the other two hybrid methods.

Fig. 2 displays the relative error for iterates x_j determined by the three hybrid methods. The figure indicates that GMRES+ TTw can stabilize the *semiconvergence* of GMRES, but GMRES + ST and GMRES + TT still have a little *semiconvergence*.

Table 5
Arnoldi steps, relative errors and CPU time of the numerical solutions for Example 4.5.

Method		Arnoldi step	Relative error	CPU (s)
GMRES		14	$145.09 \cdot 10^{0}$	0.422
hybrid method	GMRES + ST	15	$58.38 \cdot 10^{0}$	0.689
	GMRES + TT	21	$1.72 \cdot 10^{0}$	0.944
	GMRES + TTw	19	$1.91 \cdot 10^{-1}$	0.880

Table 6
Arnoldi steps, relative errors and CPU time of the numerical solutions for Example 4.6.

Method		Arnoldi step	Relative error	CPU (s)
GMRES		10	$5.79 \cdot 10^{0}$	0.229
hybrid method	GMRES + ST	10	$4.64 \cdot 10^{0}$	0.508
	GMRES + TT	14	$9.21 \cdot 10^{-1}$	0.615
	GMRES + TTw	14	$4.36 \cdot 10^{-1}$	0.659

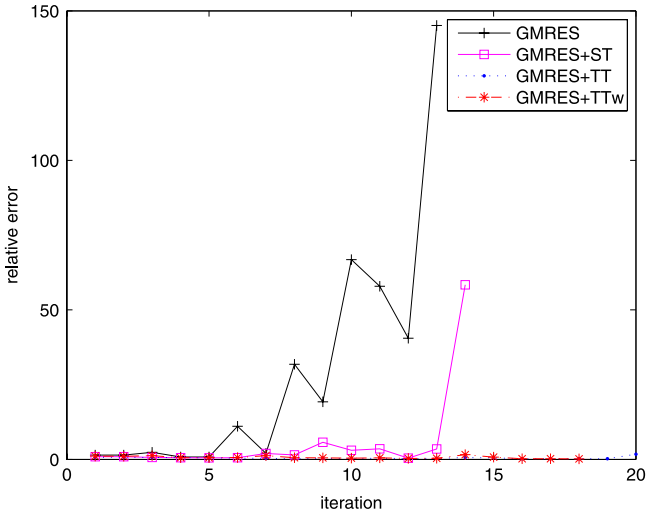

Fig. 2. Example 4.5: Norm of relative errors in iterates generated by GMRES, GMRES + ST, GMRES + TT and GMRES + TTw.

Example 4.6. The Fredholm integral equation of the first kind

$$\int_0^{\infty} K(s,t)x(t)dt = g(s), \quad s \geq 0, \tag{41}$$

with the kernel and the solution given by

$$k(s,t) := \exp(-st),$$
$$x(t) := \exp(-t/8).$$

The right-hand side function $g(s)$ is defined by (41).

We modify the code *ilaplace* from Regularization Tools [26] and discretize the integral equation by the Galerkin method with orthonormal box functions as test and trial functions, then we obtain the matrix $A \in \mathbb{R}^{2000\times 2000}$ and the discretized solution $\hat{x}$ of the error-free linear system (3). The error-free right-hand side $\hat{b}$ is given by (35). The associated contaminated vector b in (1) is obtained by adding 1% normally distributed zero mean "noise" e to $\hat{b}$; cf. (2). Thus, $\epsilon = 1 \cdot 10^{-2}$ in (36).

Table 6 reports the Arnoldi steps, the relative errors and the CPU time of Example 4.6. Neither GMRES nor GMRES + ST produce iterations with small relative errors. GMRES + TTw yields the smaller relative errors than that of GMRES + TT.

Fig. 3 displays the relative error for x_j determined by the three hybrid methods. The figure indicates that both GMRES + TT and GMRES + TTw can stabilize the *semiconvergence* of GMRES, but they still have a little *semiconvergence*.

Now, the last example illustrates the benefit of the augmentation of the generalized Krylov subspace.

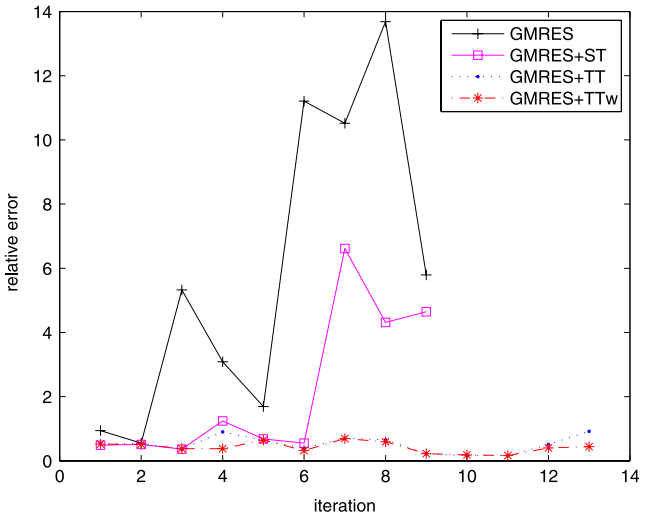

Fig. 3. Example 4.6: Norm of relative errors in iterates generated by GMRES, GMRES + ST, GMRES + TT and GMRES + TTw.

Table 7
Relative errors and CPU time of the numerical solutions without augmentation for Example 4.7.

Method	Relative error	CPU (s)
ST ($L_\mu = \mu I$)	$2.90 \cdot 10^{-1}$	0.145
TT (L_μ defined by (10))	$2.81 \cdot 10^{-1}$	0.141
TTw (L_μ defined by (17))	$2.79 \cdot 10^{-1}$	0.145

Example 4.7. Consider the Fredholm integral equation of the first kind

$$\int_0^1 K(s,t)x(t)dt = g(s), \quad 0 \le s \le 1, \tag{42}$$

with the kernel and the solution given by

$$k(s,t) := \begin{cases} s(t-1), & s < t, \\ t(s-1), & s \ge t, \end{cases}$$
$$x(t) := t.$$

The right-hand side function $g(s)$ is defined by (42). This integral equation is discussed by Delves and Mohamed [30].

We discretize the integral equation by the Galerkin method with orthonormal box functions as test and trial functions by the MATLAB program *deriv*2 from Regularization Tools [26] and obtain the matrix $A \in \mathbb{R}^{200\times 200}$ and the discretized solution $\tilde{x}$ of the error-free linear system (3). The associated contaminated vector b in (1) is obtained by adding 5% normally distributed zero mean "noise" e to $\hat{b}$; cf. (2). Thus, $\epsilon = 5 \cdot 10^{-2}$ in (36).

We first compute an approximate solution by using the three direct methods ST, TT and TTω.

A more accurate approximation to $\hat{x}$ can be computed by splitting the problem as described in Section 3.1. Define $W \in \mathbb{R}^{200\times 3}$ through the QR-factorization of

$$\hat{W} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ \vdots & \vdots & \vdots \\ 1 & 200 & 200^2 \end{pmatrix}, \qquad \hat{W} = W\hat{R}, \tag{43}$$

i.e., W is orthonormal in columns and $\hat{R} \in \mathbb{R}^{3\times 3}$ is upper triangular.

Tables 7 and 8 show that the augmentation improves the quality of the computed approximate solution and reduces the CPU time. TTw achieves the best approximate solution both with and without augmentation, while the gain for decomposition method is larger.

Table 8
Relative errors and CPU time of the numerical solutions augmented with W given by (43) for Example 4.7.

Decomposition method with W in (43)	Relative error	CPU (s)
ST ($L_\mu = \mu I$)	$1.25 \cdot 10^{-2}$	0.137
TT (L_μ defined by (10))	$1.50 \cdot 10^{-2}$	0.143
TTw (L_μ defined by (17))	$7.90 \cdot 10^{-3}$	0.140

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at http://dx.doi.org/10.1016/j.cam.2015.04.011.

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