MODIFIED TRUNCATED RANDOMIZED SINGULAR VALUE DECOMPOSITION (MTRSVD) ALGORITHMS FOR LARGE SCALE DISCRETE ILL-POSED PROBLEMS WITH GENERAL-FORM REGULARIZATION

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Abstract. In this paper, we propose new randomization based algorithms for large scale linear discrete ill-posed problems with general-form regularization: \( \min_{x} \| Lx \| \text{ subject to } \min_{x} \| Ax - b \| \), where \( L \) is a regularization matrix. Our algorithms are inspired by the modified truncated singular value decomposition (MTSVD) method, which suits only for small to medium scale problems, and randomized SVD (RSVD) algorithms that generate good low rank approximations to \( A \). We use rank-\( k \) truncated randomized SVD (TRSVD) approximations to \( A \) by truncating the rank-(\( k + q \)) RSVD approximations to \( A \), where \( q \) is an oversampling parameter. The resulting algorithms are called modified TRSVD (MTRSVD) methods. At every step, we use the LSQR algorithm to solve the resulting inner least squares problem, which is proved to become better conditioned as \( k \) increases so that LSQR converges faster. We present sharp bounds for the approximation accuracy of the RSVDs and TRSVDs for severely, moderately and mildly ill-posed problems, and substantially improve a known basic bound for TRSVD approximations. We prove how to choose the stopping tolerance for LSQR in order to guarantee that the computed and exact best regularized solutions have the same accuracy. Numerical experiments illustrate that the best regularized solutions by MTRSVD are as accurate as the ones by the truncated generalized singular value decomposition (TGSVD) algorithm, and at least as accurate as those by some existing truncated randomized generalized singular value decomposition (TRGSD) algorithms.

Key words. MTRSVD, RSVD, TRSVD, TGSVD, discrete ill-posed, general-form regularization, Lanczos bidiagonalization, LSQR

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1. Introduction. Consider the solution of the large-scale linear discrete ill-posed problem

\[
\min_{x \in \mathbb{R}^n} \| Ax - b \| \quad \text{or} \quad Ax = b, \quad A \in \mathbb{R}^{m \times n}, \quad b \in \mathbb{R}^m,
\]

where the norm \( \| \cdot \| \) is the 2-norm of a vector or matrix, the matrix \( A \) is ill conditioned with its singular values decaying to zero with no obvious gap between consecutive ones, and the right-hand side \( b = b_{\text{true}} + e \) is noisy and assumed to be contaminated by a white noise \( e \), which may stem from measurement, truncation or discretization errors, where \( b_{\text{true}} \) represents the unknown noise-free right-hand side and \( \| e \| < \| b_{\text{true}} \| \). Such kind of problem arises in a variety of applications, such as computerized tomography, electrocardiography, image deblurring, signal processing, geophysics, heat propagation, biomedical and optical imaging, groundwater modeling, and many others; see, e.g., [1, 3, 5, 6, 22, 25, 29].

The naive solution \( x_{\text{naive}} = A^\dagger b \) is a meaningless approximation to the true solution \( x_{\text{true}} = A^\dagger b_{\text{true}} \) since \( b \) is contaminated by the noise and \( A \) is extremely ill conditioned, where \( \dagger \) denotes the Moore-Penrose inverse of a matrix. Therefore, one has to use regularization to obtain a best possible approximation to \( x_{\text{true}} \) [12, 14].

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One of the common regularization approaches is to solve the standard-form regularization problem
\begin{equation}
\min \|x\| \quad \text{subject to} \quad \|Ax-b\| = \text{min}.
\end{equation}

The truncated singular value decomposition (TSVD) method is one of the most popular regularization methods for solving (1.2). The method computes a minimum 2-norm least squares solution, i.e., the TSVD solution \(x_k\), which solves the problem
\begin{equation}
\min \|x\| \quad \text{subject to} \quad x \in S_k = \{x \mid \|A_kx-b\| = \text{min}\}
\end{equation}
starting with \(k = 1\) onwards until a best regularized solution is found at some \(k\), where \(A_k\) is a best rank-\(k\) approximation to \(A\) with respect to the 2-norm and the index \(k\) plays the role of the regularization parameter. It is known from, e.g., [8], p. 79, that
\begin{equation}
\|A - A_k\| = \sigma_{k+1},
\end{equation}
where \(\sigma_{k+1}\) is the \((k + 1)\)th large singular value of \(A\). (1.2) is equivalent to the standard-form Tikhonov regularization problem
\begin{equation}
\min_{x \in \mathbb{R}^n} \left\{ \|Ax-b\|^2 + \lambda^2 \|x\|^2 \right\}
\end{equation}
with the regularization parameter \(\lambda > 0\). (1.2) amounts to (1.5) in the sense that for any regularization parameter \(\lambda \in [\sigma_n, \sigma_1]\) there is a truncation parameter \(k\) such that the solutions computed by the TSVD method and the Tikhonov regularization method are close. Furthermore, with the optimal parameter \(\lambda_{opt}\) chosen, the best regularized solutions obtained by the two methods have very comparable accuracy with essentially the minimum 2-norm error [12, 14].

Hansen [12] points out that, in many applications, minimizing the 2-norm of the solution, i.e., \(\min \|x\| = \min \|I_nx\|\) with \(I_n\) being the \(n \times n\) identity matrix, is not an optimal choice. On the one hand, \(\|x\|\) may not always be affected as much by the errors as the 2-norm of a derivative of the solution. On the other hand, the SVD basis vectors may not be well suited for computing a good regularized solution to (1.1), but choosing a regularization matrix \(L \neq I_n\) can often lead to a much better approximate solution. He presents some examples such as data approximation by bivariate spline [4]. Kilmer et al. [23] also give some examples from geophysics and heat distribution, where choosing an \(L \neq I_n\) appears more effective.

In this paper, we consider to exploit the priori information on \(x_{true}\) by using \(\min \|Lx\|\) in (1.2) and (1.3) other than \(\min \|x\|\), that is, we solve the general-form regularization problem
\begin{equation}
\min \|Lx\| \quad \text{subject to} \quad \|Ax-b\| = \text{min},
\end{equation}
where \(L \in \mathbb{R}^{p \times n}\) is usually a discrete approximation of some derivative operators. When \(L \neq I_n\), (1.5) becomes the general-form Tikhonov regularization problem
\begin{equation}
\min_{x \in \mathbb{R}^n} \left\{ \|Ax-b\|^2 + \lambda^2 \|Lx\|^2 \right\},
\end{equation}
which is equivalent to (1.6). The solution to (1.7) is unique for a given \(\lambda > 0\) when
\[\mathcal{N}(A) \cap \mathcal{N}(L) = 0 \iff \text{rank} \begin{pmatrix} A \\ L \end{pmatrix} = n,\]
where $\mathcal{N}(\cdot)$ denotes the null space of a matrix. In practical applications, $L$ is typically chosen as

$$L_1 = \begin{pmatrix} 1 & -1 & & & \\ -1 & 1 & -1 & & \\ & \ddots & \ddots & \ddots \\ & & 1 & -1 & \\ & & & & 1 \end{pmatrix} \in \mathbb{R}^{(n-1)\times n},$$

(1.8)

$$L_2 = \begin{pmatrix} -1 & 2 & -1 & & & \\ 2 & -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \ddots \\ & & 2 & -1 & 2 & -1 & \\ & & & & -1 & 2 \end{pmatrix} \in \mathbb{R}^{(n-2)\times n},$$

(1.9)

or

$$L_3 = \begin{pmatrix} L_1 \\ L_2 \end{pmatrix} \in \mathbb{R}^{(2n-3)\times n},$$

(1.10)

where $L_1$ and $L_2$ are scaled discrete approximations of the first and second derivative operators in one dimensional Fredholm integral equations of the first kind, respectively. For the corresponding $L_1$ and $L_2$ in two dimensional problems, see Section 8.2 of [14].

For small to medium scale problems, adapting the TSVD method to Problem (1.6), Hansen et al. [16] propose a modified truncated SVD (MTSVD) method that solves

$$\begin{aligned}
\min \|Lx\| \quad \text{subject to} \quad x \in S_k = \{x \mid \|A_kx - b\| = \min\}
\end{aligned}$$

(1.11)

starting with $k = 1$ onwards until a best regularized solution is found for some $k$. As in the TSVD method, $k$ plays the role of the regularization parameter. This approach is an alternative to the TGSVD method for solving (1.7). The algorithm first computes the SVD of $A$ and then extracts the best rank-$k$ approximation $A_k$ to $A$ by truncating the SVD of $A$. It solves a sequence of least squares problems by the adaptive QR factorization from $k = 1$ onwards until a best regularized solution is found. This algorithm avoids computing the GSVD of the matrix pair $\{A, L\}$, but it is not suitable for large scale problems since computing the SVD of $A$ is infeasible for $A$ large.

For $L = I_n$, Xiang and Zou [33] adapt some basic randomized algorithms from [11] to (1.5) and develop a randomized SVD (RSVD) algorithm. RSVD acts $A$ on a Gaussian random matrix to capture the dominant information on the range of $A$, and computes the SVD of a small matrix. By the SVD of the small matrix, one then obtains an approximate SVD of $A$. Halko et al. [11] have given an accuracy analysis on the randomized algorithm and approximate SVD, and have established a number of error bounds for them. Randomized algorithms have been receiving high attention in recent years and widely used in a variety of low rank approximations; see, e.g., [9, 10, 11, 24, 27, 28, 31, 32, 33, 34].

For $L \neq I_n$, Xiang and Zou [34] present a randomized GSVD (RGSVD) algorithm to solve (1.7). First, they compute a RSVD of $A$. Then they compute the GSVD of the matrix pair $\{AQ, LQ\}$, where $Q$ is the right singular vectors in RSVD. The matrix $Q$ captures the information on dominant right singular vectors of $A$, which
ensures that $AQ$ captures the dominant left singular vectors of $A$. Indeed, $AQQ^T$ is a good low rank approximation to $A$ with high probability; see [11] for some bounds and next section for refined bounds. However, the generation of $Q$ does not make use of any information on $L$. As a consequence, there is no guarantee that the GSVD of the matrix pair $(AQ, LQ)$ well approximates the dominant GSVD components of $(A, L)$, which is a critical requirement that RGSVD can obtain a good regularized solution to (1.1).

Wei et al. [32] propose new RGSVD algorithms. For the underdetermined case, their algorithm is the same as Xiang and Zou [34] in theory. An algorithmic difference is that they do not compute an approximate SVD of $A$. Instead, they compute the GSVD of the matrix pair $(AQ, LQ)$, where $Q$ captures only the information on dominant right singular vectors of $A$ and has nothing to do with $L$. Therefore, it has the same deficiency as the algorithm in [34], as mentioned above. For the overdetermined case, their RGSVD method needs to compute the GSVD of the matrix pair $(B, L)$, where $B = Q^TA \in \mathbb{R}^{l \times n}$ is a dense matrix with $Q$ being an $m \times l$ orthonormal matrix generated by randomized algorithms, $L \in \mathbb{R}^{p \times n}$ and the parameter $l$ satisfies $l + p \geq n$. Since this algorithm captures the dominant information on $A$ and retains $L$ itself, it works theoretically for (1.1). However, for a large scale (1.1), $n$ must be large, so is the size of the matrix pair $(B, L)$. This leads to the computation and storage memory of the GSVD of the matrix pair $(B, L)$ impractical because one must compute a large dense $n \times n$ matrix and invert it to obtain the right singular vector matrix of this matrix pair when using the resulting RGSVD to solve (1.6) or (1.7). As a result, the proposed RGSVD algorithm actually does not suit for large scale problems.

In this paper, inspired by the idea of randomized algorithms and the MTSVD method, we will propose a modified truncated randomized SVD (MTRSVD) method for solving (1.6). Our method consists of four steps: first, use the RSVD algorithms [11] to obtain approximate SVDs of $A$ for the underdetermined and overdetermined cases, respectively; second, truncate the approximate SVDs to obtain rank-$k$ TRSVD approximations $\tilde{A}_k$ to $A$; third, use $\tilde{A}_k$ to replace the best rank-$k$ approximation $A_k$ in (1.11); finally, solve

$$\min \|Lx\| \quad \text{subject to} \quad x \in S_k = \{x \mid \|\tilde{A}_k x - b\| = \min\}$$

starting with $k = 1$ onwards until a best regularized solution is found for some $k$. As will be seen later, this step gives rise to a large least squares problem that is different from the one in [16] and cannot be solved by adaptive QR factorizations any more because of its large size and the unavailability of the SVD of $A$. We will use the LSQR algorithm [30] to iteratively solve the resulting least squares problem.

We consider a number of theoretical issues on the MTRSVD algorithms. For severely, moderately and mildly ill-posed problems [12, 14, 18], we establish some sharp error bounds for the approximation error $\|A - QQ^T A\|$ (or $\|A - AQQ^T\|$) in terms of $\sigma_{k+1}$, where $QQ^T A$ (or $AQQ^T$) is the rank-$(k + q)$ RSVD approximation and $Q \in \mathbb{R}^{m \times (k+q)}$ (or $Q \in \mathbb{R}^{n \times (k+q)}$) is an orthonormal matrix with $q$ being an oversampling parameter. Hallo et al. [11] have presented a number of error bounds for the approximation errors. Their bounds have been used in, e.g., [32, 34] and are good enough for a nearly rank deficient $A$, but turn out to be possibly meaningless for ill-posed problems since they are pessimistic and even may never become small for any $k$ and $q$. In contrast, our bounds are always meaningful and much sharper for the aforementioned three kinds of ill-posed problems. Next, for the truncated rank-$k$ approximations $\tilde{A}_k$, we focus on a basic bound in [11] and improve it substantially.
Our new bounds are unconditionally superior to and can be much sharper than the bound for \( \tilde{A}_k \) in [11], and they explain why the error introduced in truncation step is not so damaging, an important concern in [11, Remark 9.1]. For the MTRSVD algorithms, we analyze the conditioning of the resulting inner least squares problem at each step \( k \). We will prove that the condition number monotonically decreases as \( k \) increases, such that for the same stopping tolerance the LSQR algorithm for solving it generally converges faster and uses fewer inner iterations as \( k \) increases.

In the meantime, we consider efficient implementations of Lanczos bidiagonalization used within LSQR for the inner least squares problems. Importantly, we will make a detailed analysis on the stopping tolerance for LSQR, showing how to choose it so as to guarantee that the computed and exact best regularized solution have the same accuracy. We prove that the stopping tolerance for LSQR is not restrictive and a reasonably small one is good enough, provided that the regularization matrix \( L \) is well conditioned. Finally, we report numerical experiments to illustrate the generality and effectiveness of our algorithms. We show that, for the \( m \geq n \) case with \( n \) not large, the best regularized solutions obtained by MTRSVD are as accurate as those by the TGSVD algorithm and the TRGSVD algorithm in [32]. When \( n \) is large, the TRGSVD algorithm in [32] is out of memory in our computer, but our algorithm works well. For the \( m \leq n \) case, the best regularized solutions by MTRSVD are very comparable to those by the TGSVD algorithm and are at least as accurate as those by the TRGSVD algorithms in [32, 34].

Our paper is organized as follows. In Section 2, we review the RSVD algorithms and establish new error bounds for the RSVD approximations to \( A \) for severely, moderately and mildly ill-posed problems, respectively. In Section 3, we present the MTRSVD algorithms, establish new sharp bounds for the TRSVD approximation to \( A \), and make an analysis on the conditioning of inner least squares problems and on the stopping tolerance for LSQR. In Section 4, we report numerical examples to illustrate that our algorithms work well. Finally, we conclude the paper in Section 5.

2. RSVD and sharp error bounds. Let the compact SVD of \( A \in \mathbb{R}^{m \times n} \) be

\[
A = U \Sigma V^T,
\]

where \( U = (u_1, u_2, \ldots, u_s) \in \mathbb{R}^{m \times s} \) and \( V = (v_1, v_2, \ldots, v_s) \in \mathbb{R}^{n \times s} \) are column orthonormal, \( \Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_s) \in \mathbb{R}^{s \times s} \) with \( s = \min\{m, n\} \) and \( \sigma_1, \sigma_2, \ldots, \sigma_s \) being the singular values and labeled as \( \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_s > 0 \). Then

\[
A_k = U_k \Sigma_k V_k^T
\]

is one of the best rank-\( k \) approximations to \( A \) with respect to the 2-norm, where \( U_k = (u_1, u_2, \ldots, u_k) \in \mathbb{R}^{m \times k} \) and \( V_k = (v_1, v_2, \ldots, v_k) \in \mathbb{R}^{n \times k} \) are column orthonormal, and \( \Sigma_k = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_k) \in \mathbb{R}^{k \times k} \). Define the condition number of \( A \) as

\[
\kappa(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)} = \frac{\sigma_1}{\sigma_s}.
\]

The following Algorithm 1 is the basic randomized algorithm, presented in [11], that computes a low rank approximation to \( A \) with an approximate SVD of \( A \) for the overdetermined case \( (m \geq n) \).

The mechanism of Algorithm 1 is as follows: the information of the column space of \( A \) is extracted in step 2, i.e., \( \mathcal{R}(Y) \subseteq \mathcal{R}(A) \) where \( \mathcal{R}(\cdot) \) denotes the column space or range of a matrix. It is clear that the columns of \( Q \) span the main range of \( A \) in
Algorithm 1 (RSVD) Given $A \in \mathbb{R}^{m \times n}$ ($m \geq n$), $l = k + q < n$ and $q \geq 4$, compute an approximate SVD: $A \approx \tilde{U}\tilde{\Sigma}\tilde{V}^T$ with $\tilde{U} \in \mathbb{R}^{m \times l}$, $\tilde{\Sigma} \in \mathbb{R}^{l \times l}$ and $\tilde{V} \in \mathbb{R}^{n \times l}$.

1: Generate an $n \times l$ Gaussian random matrix $\Omega$.
2: Form the $m \times l$ matrix $Y = A\Omega$.
3: Compute the $m \times l$ orthonormal matrix $Q$ via QR factorization $Y = QR$.
4: Form the $l \times n$ matrix $B = Q^TA$.
5: Compute the compact SVD of the small matrix $B$: $B = W\hat{\Sigma}\hat{V}^T$.
6: Form the $m \times l$ matrix $\tilde{U} = QW$, and $A \approx \tilde{U}\hat{\Sigma}\hat{V}^T = QQ^TA$.

Step 3 and $\mathcal{R}(Q) = \mathcal{R}(Y) \subseteq \mathcal{R}(A)$. Noting $\mathcal{R}(A) = \mathcal{R}(U)$, the factor $Q$ captures the dominant left singular vectors of $A$. In step 4, because of $\mathcal{R}(B^T) \subseteq \mathcal{R}(A^T) = \mathcal{R}(V)$, the matrix $B$ provides information on the dominant right singular vectors of $A$. In step 6, the algorithm modifies the approximate left singular vectors.

For the underdetermined case ($m \leq n$), Halko et al. [11] present Algorithm 2, which is equivalent to applying Algorithm 1 to $A^T$.

Algorithm 2 (RSVD) Given $A \in \mathbb{R}^{m \times n}$ ($m \leq n$), $l = k + q < m$ and $q \geq 4$, compute an approximate SVD: $A \approx \tilde{U}\tilde{\Sigma}\tilde{V}^T$ with $\tilde{U} \in \mathbb{R}^{m \times l}$, $\tilde{\Sigma} \in \mathbb{R}^{l \times l}$ and $\tilde{V} \in \mathbb{R}^{n \times l}$.

1: Generate an $l \times m$ Gaussian random matrix $\Omega$.
2: Form the $l \times n$ matrix $Y = \Omega A$.
3: Compute the $n \times l$ orthonormal matrix $Q$ via QR factorization $Y^T = QR$.
4: Form the $m \times l$ matrix $B = AQ$.
5: Compute the compact SVD of the small matrix $B$: $B = \hat{U}\hat{\Sigma}\hat{V}^T$.
6: Form the $n \times l$ matrix $\tilde{V} = QW$, and $A \approx \tilde{U}\hat{\Sigma}\hat{V}^T = AQQ^T$.

When $q \geq 4$, Halko et al. [11] establish the following basic estimate on the approximation accuracy of $QQ^TA$ generated by Algorithm 1:

\[(2.3) \quad \|A - QQ^TA\| \leq \left(1 + 6\sqrt{(k + q)q\log q}\right)\sigma_{k+1} + 3\sqrt{k + q}\left(\sum_{j > k} \sigma_j^2\right)^{1/2}\]

with failure probability at most $3q^{-q}$. Based on (2.3), Halko et al. [11] derive a simplified elegant error bound

\[(2.4) \quad \|A - QQ^TA\| \leq \left(1 + 9\sqrt{(k + q)(n - k)}\right)\sigma_{k+1}\]

with failure probability at most $3q^{-q}$. As we can see clearly, for a fixed $k$ the above two bounds monotonically increases with $q$, which is not in accordance with a basic result that, for a fixed $k$, the left hand side of (2.4) monotonically decreases with $q$; see Proposition 8.5 of [11]. Xiang and Zou [33] and Wei et al. [32] directly exploit the bound (2.4) in their analysis. For a nearly rank deficient $A$, the monotonic increasing property of the right-hand sides of (2.3) and (2.4) with $q$ do not have serious harm since the bound can be small enough to detect the numerical rank $k$ whenever $q$ is not large, the singular values $\sigma_k \gg \sigma_{k+1}$ and $\sigma_{k+1}$ is numerically small. In the context of ill-posed problems, however, the situation is completely different since the bound (2.4) may be too pessimistic and meaningless, as will be clear soon.
We notice another basic bound from [11] that has received little attention but appears more insightful and useful than (2.3), at least in the context of ill-posed problems:

\[ \|A - QQ^T A\| \leq \left( 1 + 16 \sqrt{\frac{1 + \frac{k}{q+1}}{\frac{k}{q+1}}} \right) \sigma_{k+1} + \frac{8\sqrt{k+q}}{q+1} \left( \sum_{j>k} \sigma_j^2 \right)^{1/2} \]

with failure probability at most \(3e^{-q}\).

In the manner of deriving (2.4) from (2.3), we have a simplified form of (2.5):

\[ \|A - QQ^T A\| \leq \left( 1 + 16 \sqrt{\frac{1 + \frac{k}{q+1}}{\frac{k}{q+1}}} + \frac{8\sqrt{(k+q)(n-k)}}{q+1} \right) \sigma_{k+1}. \]

On contrary to (2.3) and (2.4), an advantage of the bounds (2.5) and (2.6) is that they monotonically decrease with \(q\) for a given \(k\). Compared with (2.3), a minor theoretical disadvantage of (2.5) is that its failure probability \(3e^{-q}\) is a little higher than \(3q^{-q}\) of (2.3) for \(q \geq 4\). But this should not cause any essential problem for practical purposes.

For the bound (2.6), it is easily justified that the factor in front of \(\sigma_{k+1}\) lies between \(1 + \mathcal{O}(\sqrt{n})\) and \(1 + \mathcal{O}(n)\) for a small fixed \(q\), and it is \(1 + \mathcal{O}(\sqrt{n})\) for \(k\) not big when dynamically choosing \(q = k\) roughly. In contrast, for the bound (2.4), the factor in front of \(\sigma_{k+1}\) ranges from \(1 + \mathcal{O}(\sqrt{n})\) to \(1 + \mathcal{O}(n)\) for any \(q\).

We will show that the bounds (2.4) and (2.6) may be fatal overestimates in the context of ill-posed problems. Based on (2.5) and following Jia’s works [19, 20], we carefully analyze the approximation accuracy of \(QQ^T A\) for three kinds of ill-posed problems: severely, moderately and mildly ill-posed problems, and establish much more accurate bounds.

Before proceeding, we first give a precise characterization of the degree of ill-posedness of (1.1) which was introduced in [18] and has been widely used in, e.g., the books [1, 7, 12, 14, 26].

**Definition 2.1.** If \(\sigma_j = \mathcal{O}(\rho^{-j})\), \(j = 1, 2, \ldots, n\) with \(\rho > 1\), then (1.1) is severely ill-posed. If the singular values \(\sigma_j = \mathcal{O}(\rho^{-j})\), \(j = 1, 2, \ldots, n\), then (1.1) is mildly or moderately ill-posed for \(\frac{1}{2} < \alpha \leq 1\) or \(\alpha > 1\).

We mention that the requirement \(\alpha > \frac{1}{2}\) does not appear in the aforementioned books but it is added in [19, 20], where it is pointed out that this requirement is naturally met when the kernel of an underlying linear Fredholm equation of the first kind is square integrable over a defined domain.

Keep in mind that the factors in front of \(\sigma_{k+1}\) in (2.4) and (2.6) lie between \(1 + \mathcal{O}(\sqrt{n})\) and \(1 + \mathcal{O}(n)\) for a given \(k\). However, for moderately and mildly ill-posed problems, the bounds (2.4) and (2.6) may never be small for \(k\) not big and \(\alpha\) close to one; for \(\alpha\) close to \(\frac{1}{2}\), they are definitely not small as \(k\) increases up to \(n - q - 1\). These bounds, if realistic, mean that Algorithm 1 may never generate a meaningful rank-\((k+q)\) approximation to \(A\). Fortunately, as we will show below, the bound (2.6) can be improved substantially for the three kinds of ill-posed problems, and the new bounds indicate that Algorithm 1 (or Algorithm 2) indeed generates very accurate rank-\((k+q)\) approximations to \(A\).

**Theorem 2.2.** For the severely ill-posed problems with \(\sigma_j = \mathcal{O}(\rho^{-j})\) and \(\rho > 1\),
\( j = 1, 2, \ldots, n, \) it holds that

\[
\|A - QQ^T A\| \leq \left(1 + 16 \sqrt{1 + \frac{k}{q + 1}} + \frac{8 \sqrt{k + q}}{q + 1} (1 + \mathcal{O}(\rho^{-2}))\right) \sigma_{k+1}
\]

with failure probability at most \( 3e^{-q} \) for \( q \geq 4 \) and \( k = 1, 2, \ldots, n - q - 1 \).

**Proof.** By the assumption on the singular values \( \sigma_j \), we obtain

\[
\left( \sum_{j=k+1}^{n} \sigma_j^2 \right)^{1/2} = \sigma_{k+1} \left( \sum_{j=k+1}^{n} \frac{\sigma_j^2}{\sigma_{k+1}^2} \right)^{1/2} = \sigma_{k+1} \left( 1 + \sum_{j=k+2}^{n} \frac{\sigma_j^2}{\sigma_{k+1}^2} \right)^{1/2}
\]

\[
= \sigma_{k+1} \left( 1 + \sum_{j=k+2}^{n} \mathcal{O}(\rho^{2(k-j)+2}) \right)^{1/2}
\]

\[
= \sigma_{k+1} \left( 1 + \mathcal{O} \left( \sum_{j=k+2}^{n} \rho^{2(k-j)+2} \right) \right)^{1/2}
\]

\[
= \sigma_{k+1} \left( 1 + \mathcal{O} \left( \rho^{2} \left( 1 - \rho^{-2(2n-k-1)} \right) \right) \right)^{1/2}
\]

\[
= \sigma_{k+1} \left( 1 + \mathcal{O}(\rho^{-2}) \right)^{1/2}
\]

\[
= \sigma_{k+1} \left( 1 + \mathcal{O}(\rho^{-2}) \right) .
\]

Substituting (2.8) into (2.5) gives (2.7).

**Theorem 2.3.** For the moderately and mildly ill-posed problems with \( \sigma_j = \zeta j^{-\alpha} \), \( j = 1, 2, \ldots, n \), where \( \alpha > 1/2 \) and \( \zeta > 0 \) is some constant, it holds that

\[
\|A - QQ^T A\| \leq \left(1 + 16 \sqrt{1 + \frac{k}{q + 1}} + \frac{8 \sqrt{k + q}}{q + 1} \sqrt{\frac{k}{2\alpha - 1}} \left(\frac{k+1}{k}\right)^{\alpha}\right) \sigma_{k+1}
\]

with failure probability at most \( 3e^{-q} \) for \( q \geq 4 \) and \( k = 1, 2, \ldots, n - q - 1 \).

**Proof.** By the assumption on the singular values \( \sigma_j \), we obtain

\[
\left( \sum_{j=k+1}^{n} \sigma_j^2 \right)^{1/2} = \sigma_{k+1} \left( \sum_{j=k+1}^{n} \frac{\sigma_j^2}{\sigma_{k+1}^2} \right)^{1/2}
\]

\[
= \sigma_{k+1} \left( \sum_{j=k+1}^{n} \left( \frac{j}{k+1} \right)^{-2\alpha} \right)^{1/2}
\]

\[
= \sigma_{k+1} \left( (k+1)^{2\alpha} \sum_{j=k+1}^{n} \frac{1}{j^{2\alpha}} \right)^{1/2}
\]

\[
< \sigma_{k+1}(k+1)^{\alpha} \left( \int_{k}^{\infty} \frac{1}{x^{2\alpha}} dx \right)^{1/2} \quad \text{due to} \quad \alpha > \frac{1}{2}
\]

\[
= \sigma_{k+1} \left( \frac{k+1}{k} \right)^{\alpha} \sqrt{\frac{k}{2\alpha - 1}}.
\]
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Substituting (2.10) into (2.5) proves (2.9). □

From Theorems 2.2–2.3, it is easy to see that the error bounds (2.7) and (2.9) decrease with the oversampling number \(q\). Importantly, whenever we take \(q = k\) roughly, the factors in front of \(\sigma_{k+1}\) in (2.7) and (2.9) reduce to \(O(1)\), independent of \(n\), provided that \(\alpha\) is not close to \(\frac{1}{2}\). On the other side, for a fixed small \(q \geq 4\), the factors in front of \(\sigma_{k+1}\) in (2.7) and (2.9) are \(1 + O(\sqrt{T})\) and \(1 + O(k)\) for \(\alpha\) not close to one, respectively, meaning that the rank-\((k + q)\) approximation to \(A\) may be more accurate for severely ill-posed problems than for moderately and mildly ill-posed problems. For a fixed \(k\), the bigger \(q\), the smaller the bounds (2.7) and (2.9), i.e., the more accurate the rank-\(k\) RSVD approximations. As a result, in any event, our new bounds are much sharper than (2.4) and (2.6), and get more insight into the accuracy of rank-(\(k + q\)) approximations for \(k\) not big and \(\alpha\) not close to \(\frac{1}{2}\), where the factors in front of \(\sigma_{k+1}\) has been shown to lie between \(1 + O(\sqrt{n})\) and \(1 + O(n)\).

Finally, we mention that all the results on \(\|A - QQ^T\|\) in this section apply to \(\|A - AQQ^T\|\) as well, where \(AQQ^T\) is generated by Algorithm 2.

3. TRSVD and error bounds, and the MTRSV algorithms and their analysis. We consider the MTRSV method and compute the MTRSV solutions \(x_{L,k}\) to the problem (1.12) starting with \(k = 1\). The MTRSV solutions \(x_{L,k}\) are regularized solutions to the general-form regularization problem (1.6). MTRSV first extracts a rank-\(k\) TRSVD approximation \(A_k\) from \(QQ^T A\) (or \(AQQ^T\)) to \(A\), and then utilizes the LSQR algorithm [30] to iteratively solve the resulting least squares problem at each iteration \(k\) in (1.12). This step is called inner iteration. Starting with \(k = 1\), MTRSV proceeds until a best regularized solution is found at some \(k = k_0\), at which the semi-convergence of MTRSV occurs, namely, the error \(\|L(x_{L,k} - x_{true})\|\) decreases as \(k\) increases up to \(k_0\) and then increases after \(k > k_0\).

Recall that Algorithm 1 generates a rank-\(l\) approximation \(UU^T\) to \(A\). Let

\[
\tilde{U} = (\tilde{u}_1, \tilde{u}_2, \ldots, \tilde{u}_l) \in \mathbb{R}^{m \times l}, \quad \tilde{V} = (\tilde{v}_1, \tilde{v}_2, \ldots, \tilde{v}_l) \in \mathbb{R}^{n \times l}
\]

and

\[
\tilde{\Sigma} = \text{diag}(\tilde{\sigma}_1, \tilde{\sigma}_2, \ldots, \tilde{\sigma}_l) \in \mathbb{R}^{l \times l}
\]

with \(\tilde{\sigma}_1 \geq \tilde{\sigma}_2 \geq \cdots \geq \tilde{\sigma}_l > 0\). Take

\[
(3.1) \quad \tilde{U}_k = (\tilde{u}_1, \tilde{u}_2, \ldots, \tilde{u}_k) \in \mathbb{R}^{m \times k}, \quad \tilde{V}_k = (\tilde{v}_1, \tilde{v}_2, \ldots, \tilde{v}_k) \in \mathbb{R}^{n \times k},
\]

and

\[
\tilde{\Sigma}_k = \text{diag}(\tilde{\sigma}_1, \tilde{\sigma}_2, \ldots, \tilde{\sigma}_k) \in \mathbb{R}^{k \times k},
\]

and form

\[
(3.2) \quad \tilde{A}_k = \tilde{U}_k \tilde{\Sigma}_k \tilde{V}_k^T,
\]

which is the best rank-\(k\) approximation to \(UU^T = QQ^T A\), called a rank-\(k\) TRSVD approximation to \(A\). Halko et al. [11] prove the following basic result.

**Theorem 3.1.** Let \(\tilde{A}_k\) be the rank-\(k\) TRSVD approximation to \(A\) defined by (3.2). Then the approximation error is

\[
(3.3) \quad \|A - \tilde{A}_k\| \leq \sigma_{k+1} + \|A - QQ^T A\|.
\]
The bound (3.3) reflects the worse case. In Remark 9.1, Halko et al. [11] point out that “In the randomized setting, the truncation step appears to be less damaging than the error bound of Theorem 9.3 (i.e., (3.3) here) suggests, but we currently lack a complete theoretical understanding of its behavior.” That is to say, the first term \( \sigma_{k+1} \) in (3.3) is generally conservative and may be reduced substantially.

Keep in mind that \( A \) has \( s \) singular values \( \sigma_i \) with \( s = \min\{m, n\} \). Jia [21] has improved (3.3) and derived sharper bounds, which explain why (3.3) may be an overestimate, as shown in the following theorem.

**Theorem 3.2 ([21]).** Let \( \tilde{A}_k \) be the rank-\( k \) TRSVD approximation to \( A \) defined by (3.2). Then it holds that

\[
\| A - \tilde{A}_k \| \leq \tilde{\sigma}_{k+1} + \| A - QQ^T A \|, \tag{3.4}
\]

where \( \tilde{\sigma}_{k+1} \) is the \((k+1)\)-th singular value of \( Q^T A \) and satisfies

\[
\sigma_{m-q+1} \leq \tilde{\sigma}_{k+1} \leq \sigma_{k+1} \tag{3.5}
\]

with the definition \( \sigma_{n+1} = \cdots = \sigma_{m} = 0 \). Analogously, for the rank-\( k \) TRSVD approximation \( \tilde{A}_k \) constructed by Algorithm 2, it holds that

\[
\| A - \tilde{A}_k \| \leq \tilde{\sigma}_{k+1} + \| A - AQQ^T \|, \tag{3.6}
\]

where \( \tilde{\sigma}_{k+1} \) is the \((k+1)\)-th singular value of \( AQ \) and satisfies

\[
\sigma_{n-q+1} \leq \tilde{\sigma}_{k+1} \leq \sigma_{k+1} \tag{3.7}
\]

with the definition \( \sigma_{n+1} = \cdots = \sigma_{n} = 0 \).

Particularly, the inequalities “\( \leq \)” become strict “\( < \)” in (3.5) and (3.7) if all the singular values \( \sigma_j \) of \( A \) are simple.

This theorem shows that the bound (3.4) is unconditionally superior to the bound (3.3) and the former can improve the latter substantially since \( \tilde{\sigma}_{k+1} \) can be much smaller than \( \sigma_{k+1} \) and even be arbitrarily close to zero whenever \( m-q+1 > n \). Once \( \tilde{\sigma}_{k+1} < \sigma_{k+1} \) considerably, the first term of (3.4) is negligible relative to the second term, and we will approximately have

\[
\| A - \tilde{A}_k \| \approx \| A - QQ^T A \|. \tag{3.8}
\]

Regarding the MTRSVD solution \( x_{L,k} \), we can establish the following result.

**Theorem 3.3.** Let \( \tilde{A}_k \) denote the rank-\( k \) TRSVD approximation to \( A \) generated by Algorithm 1 or Algorithm 2. Then the solution to (1.12) can be written as

\[
x_{L,k} = x_k - (L(I_n - \tilde{V}_k \tilde{V}_k^T)) \dagger Lx_k, \tag{3.9}
\]

where \( x_k = \tilde{A}_k^+ b \) is the minimum 2-norm solution to the least squares problem

\[
\min_{x \in \mathbb{R}^n} \| \tilde{A}_k x - b \|. \tag{3.10}
\]

**Proof.** Following Eldén [5], we have

\[
x_{L,k} = (I_n - (L(I_n - \tilde{A}_k^+ \tilde{A}_k))^+ L)\tilde{A}_k^+ b
= x_k - (L(I_n - \tilde{A}_k^+ \tilde{A}_k))^+ Lx_k. \tag{3.11}
\]
Noting (3.2), we have
\[
\tilde{A}_k^* \tilde{A}_k = \tilde{V}_k \tilde{V}_k^T.
\]
Substituting the above into (3.10), we obtain (3.8). \(\Box\)

Let \(z_k = \left( L(I_n - \tilde{V}_k \tilde{V}_k^T) \right)^\dagger Lx_k \). Then \(z_k\) is the minimum 2-norm solution to the least squares problem
\[
(3.11) \quad \min_{z \in \mathbb{R}^n} \| L(I_n - \tilde{V}_k \tilde{V}_k^T)z - Lx_k \|.
\]
We must point out that the problem (3.11) and its coefficient matrix are different from those in the MTSVD method in which the coefficient matrix is \(LV_{n-k}\) with \(V_{n-k} = (v_{k+1}, \ldots, v_n)\) available from the SVD (2.1) of \(A\).

Because of the large size of \(L(I_n - \tilde{V}_k \tilde{V}_k^T)\), we suppose that the problem (3.11) can only be solved by iterative solvers. We will use the LSQR algorithm [30] to solve the problem. In order to make full use of the sparsity of \(L\) itself and reduce the computational cost and storage memory, it is vital to avoid forming the dense matrix \(L(I_n - \tilde{V}_k \tilde{V}_k^T)\) explicitly within LSQR. Notice that the only action of \(L(I_n - \tilde{V}_k \tilde{V}_k^T)\) in the Lanczos diagonalization process and LSQR is to form the products of it and its transpose with vectors. We propose Algorithm 3, which efficiently implements the Lanczos bidiagonalization process with the starting vector \(\tilde{u}_1 = Lx_k/\|Lx_k\|\).

**Algorithm 3** \(k\)-step Lanczos bidiagonalization process on \(L(I_n - \tilde{V}_k \tilde{V}_k^T)\)

1. Taking \(\tilde{u}_1 = Lx_k/\|Lx_k\|, w_1 = L^T \tilde{u}_1, g_1 = \tilde{V}_k^T \tilde{u}_1\) and define \(\beta_1 \tilde{v}_0 = 0.\)
2. For \(j = 1, 2, \ldots, k\)
   - \(\tilde{p} = w_j - \tilde{V}_k (\tilde{V}_k^T w_j) - \beta_j \tilde{v}_{j-1}\)
   - \(\alpha_j = \|\tilde{p}\|; \quad \tilde{v}_j = \tilde{p}/\alpha_j\)
   - \(\tilde{r} = L \tilde{u}_j - L \tilde{V}_k g_j - \alpha_j \tilde{u}_j\)
   - \(\beta_{j+1} = \|\tilde{r}\|; \quad \tilde{u}_{j+1} = \tilde{r}/\beta_{j+1}\)
   - \(w_{j+1} = L^T \tilde{u}_{j+1}; \quad g_{j+1} = \tilde{V}_k^T \tilde{u}_{j+1}\)

We now consider the solution of (3.11) using LSQR. Suppose
\[
(3.12) \quad \tilde{V} = \left( \begin{array}{c} \tilde{V}_k \\ \tilde{V}_{n-k} \end{array} \right) \in \mathbb{R}^{n \times n}
\]
is an orthogonal matrix. It is then direct to obtain
\[
L(I_n - \tilde{V}_k \tilde{V}_k^T) = L\tilde{V}_{n-k} \tilde{V}_{n-k}^T.
\]
Since \(\tilde{V}_{n-k}\) is column orthonormal, the nonzero singular values of \(L\tilde{V}_{n-k} \tilde{V}_{n-k}^T\) are identical to the singular values of \(L\tilde{V}_{n-k}\). As a result, we have
\[
(3.13) \quad \kappa(L(I_n - \tilde{V}_k \tilde{V}_k^T)) = \kappa(L\tilde{V}_{n-k} \tilde{V}_{n-k}^T) = \kappa(L\tilde{V}_{n-k}).
\]
Next, we cite a lemma [8, p. 78] and exploit it to investigate how the conditioning of (3.11) changes as \(k\) increases.

**Lemma 3.4.** If \(B \in \mathbb{R}^{m \times n}, m > n\) and \(c \in \mathbb{R}^m\), then
\[
\sigma_{\max} \left( \begin{bmatrix} B & c \end{bmatrix} \right) \geq \sigma_{\max}(B),
\]
\[
\sigma_{\min} \left( \begin{bmatrix} B & c \end{bmatrix} \right) \leq \sigma_{\min}(B).
\]
This lemma shows that if a column is added to a rectangular matrix then the largest singular value increases and the smallest singular value decreases. Therefore, we directly obtain the following result on the conditioning of (3.11).

**Theorem 3.5.** Let the matrix $\tilde{V}_{n-k}$ be defined by (3.12). Then for $p \geq n-k$, we have

\begin{equation}
\kappa(L\tilde{V}_{n-k}) \geq \kappa(L\tilde{V}_{n-(k+1)}), \quad k = 1, 2, \ldots, n-1,
\end{equation}

i.e.,

\begin{equation}
\kappa(L(I_n - \tilde{V}_k\tilde{V}_k^T)) \geq \kappa(L(I_n - \tilde{V}_{k-1}\tilde{V}_{k-1}^T)), \quad k = 1, 2, \ldots, n-1.
\end{equation}

This theorem indicates that, when applied to solving (3.11), the LSQR algorithm generally converges faster with $k$ by recalling that the worst convergence factor of LSQR is $\kappa(L\tilde{V}_{n-k})+1\kappa(L\tilde{V}_{n-k})^{-1}$; see [2, p. 291]. Particularly, in exact arithmetic, LSQR will find the exact solution $z_k$ of (3.11) after at most $n-k$ iterations.

Having done the above, we can present our MTRSVD algorithm for the $m \geq n$ case, named as Algorithm 4.

**Algorithm 4 (MTRSVD)** Given $A \in \mathbb{R}^{m \times n}(m \geq n)$ and $l = k + q < n$ and $q \geq 4$, compute the solution $x_{L,k}$ of (1.12).

1. Use Algorithm 1 to compute the rank-$k$ TRSVD approximation $\tilde{A}_k$ to $A$: $\tilde{A}_k = \tilde{U}_k\tilde{\Sigma}_k\tilde{V}_k^T$.
2. Compute the the minimum 2-norm solution $x_k$ to (3.9).
3. Compute the solution $z_k$ to (3.11) by LSQR.
4. Compute the solution $x_{L,k}$, defined by (3.8), to the problem (1.12).

For the $m \leq n$ case, making use of Algorithm 2, we present Algorithm 5, a variant of Algorithm 4.

**Algorithm 5 (MTRSVD)** Given $A \in \mathbb{R}^{m \times n}(m \leq n)$ and $l = k + q < n$ and $q \geq 4$, compute the solution $x_{L,k}$ of (1.12).

1. Use Algorithm 2 to compute the rank-$k$ TRSVD approximation $\tilde{A}_k$ to $A$: $\tilde{A}_k = \tilde{U}_k\tilde{\Sigma}_k\tilde{V}_k^T$.
2. Compute the minimum 2-norm solution $x_k$ to (3.9).
3. Compute the solution $z_k$ to (3.11) by LSQR.
4. Compute the solution $x_{L,k}$, defined by (3.8), to the problem (1.12).

We comment that at step 3 of Algorithms 4–5, in numerical experiments we will use the Matlab function `lsqr.m` to solve the problems with a given tolerance `tol` as the stopping criterion. In what follows we make a detailed analysis and show that the default $tol = 10^{-6}$ is generally good enough and larger $tol$ can be allowed in practical applications.

First of all, let us estimate the accuracy of the computed solution $\bar{z}_k$ with the stopping tolerance $tol$. Let $r = Lx_k - L(I_n - \tilde{V}_k\tilde{V}_k^T)z_k$ be the residual of the solution
$z_k$ to the problem (3.11). It is known from [30] that, with the stopping tolerance $\text{tol}$, the computed $\tilde{z}_k$ is the exact solution to the perturbed problem

$$
\min_{z \in \mathbb{R}^n} \| (L(I_n - \tilde{V}_k \tilde{V}_k^T) + E_k) z - Lx_k \|,
$$

where the perturbation matrix

$$
E_k = - \frac{r_k L(I_n - \tilde{V}_k \tilde{V}_k^T)}{\| r_k \|_2},
$$

with

$$
r_k = Lx_k - L(I_n - \tilde{V}_k \tilde{V}_k^T)\tilde{z}_k
$$

being the residual of the computed solution $\tilde{z}_k$ and

$$
\| E_k \| \| L(I_n - \tilde{V}_k \tilde{V}_k^T) \| \| r_k \| \leq \text{tol}.
$$

For details on implementations, we refer to [30].

With the above notation and (3.13), defining $\eta = \text{tol} \cdot \kappa(L\tilde{V}_{n-k})$, exploiting the standard perturbation theory [17, p. 382], we obtain

$$
\| \tilde{z}_k - z_k \| \leq \text{tol} \cdot \kappa(L\tilde{V}_{n-k}) \left( 2 + (\kappa(L\tilde{V}_{n-k}) + 1) \frac{\| r_k \|}{\| L(I_n - \tilde{V}_k \tilde{V}_k^T) \| \| z_k \|} \right).
$$

Actually, by checking its proof we find that the above factor $\kappa(L\tilde{V}_{n-k}) + 1$ can be replaced by $\kappa(L\tilde{V}_{n-k})$ in our context since the left hand side $Lx_k$ in the perturbed (3.16) is unperturbed.

In applications, $L$ is typically well conditioned [12, 14]. Since $\kappa(L) \geq \kappa(L\tilde{V}_{n-k})$ for $p \geq n - k$, the left hand side of (3.17) is at least as small as $\mathcal{O}(\text{tol})$ with a generic constant in $\mathcal{O}(\cdot)$.

Recall from (3.8) that the MTRSVD solution

$$
x_{L,k} = x_k - z_k,
$$

and define the computed solution

$$
\tilde{x}_{L,k} = x_k - \tilde{z}_k.
$$

We thus have $\| x_{L,k} - \tilde{x}_{L,k} \| = \| z_k - \tilde{z}_k \|$, from which and (3.17) it is reasonable to suppose

$$
\frac{\| x_{L,k} - \tilde{x}_{L,k} \|}{\| x_{L,k} \|} \approx \frac{\| z_k - \tilde{z}_k \|}{\| z_k \|} \leq \mathcal{O}(\text{tol})
$$

since it is generally impossible that $\| x_{L,k} \|$ is much smaller or larger than $\| z_k \|$.

Let $x_{L}^{\text{opt}}$ be a best possible regularized solution to the problem (1.6) with the white noise $e$. Then under a certain necessary discrete Picard condition, a GSVD analysis indicates that the error $\| x_{L}^{\text{opt}} - x_{true} \| \geq \mathcal{O}(\| e \|)$ with a generic constant in $\mathcal{O}(\cdot)$; see [12, p. 83].
Let $x_{L,k_0}$ be the best regularized solutions by the MTRSVD algorithms. Then

$$\|x_{L,k_0} - x_{true}\| \geq \|x_{opt}^L - x_{true}\| \geq O(\|e\|).$$

(3.19)

By (3.17) and (3.18) as well as $\|x_{L,k_0}\| \approx \|x_{true}\|$, we have

$$\|\bar{x}_{L,k_0} - x_{true}\| \leq \|x_{L,k_0} - x_{true}\| \leq \|\bar{x}_{L,k_0} - x_{true}\| + O(tol).$$

(3.20)

On the other hand, we similarly obtain

$$\|\bar{x}_{L,k_0} - x_{true}\| \geq \|x_{L,k_0} - x_{true}\| - O(tol).$$

Suppose that the noise free problem of (1.1) is consistent, i.e., $Ax_{true} = b_{true}$. Since $\|A\|\|x_{true}\| \geq \|b_{true}\|$, it follows from (3.19) that

$$\|x_{L,k} - x_{true}\| \approx \|A\|\|x_{L,k} - x_{true}\| \geq \|A\|O(\frac{\|e\|}{\|b_{true}\|}) = O\left(\frac{\|e\|}{\|b_{true}\|}\right)$$

when $\|A\| \approx 1$ (this can always be done by suitable scaling). As a result, summarizing the above derivation, we have proved the following results.

**Theorem 3.6.** If $L$ is well conditioned and

$$O(tol) < \frac{\|e\|}{\|b_{true}\|},$$

(3.20)

then

$$\frac{\|\bar{x}_{L,k_0} - x_{true}\|}{\|x_{true}\|} - O(tol) \leq \frac{\|x_{L,k_0} - x_{true}\|}{\|x_{true}\|} \leq \frac{\|x_{L,k_0} - x_{true}\|}{\|x_{true}\|} + O(tol),$$

(3.21)

i.e.,

$$\frac{\|\bar{x}_{L,k_0} - x_{true}\|}{\|x_{true}\|} = \frac{\|x_{L,k_0} - x_{true}\|}{\|x_{true}\|}$$

(3.22)

within the error $O(tol)$ with a generic constant in $O(\cdot)$, meaning that the computed $\bar{x}_{L,k_0}$ has the same as the exact $x_{L,k_0}$ as an approximation to $x_{true}$.

Furthermore, based the above, we can establish general results, which include Theorem 3.6 as a special case. Since $x_{L,k_0}$’s are best possible regularized solutions by the MTRSVD algorithms, i.e.,

$$\frac{\|x_{L,k_0} - x_{true}\|}{\|x_{true}\|} = \min_{k=1,2,...,n} \frac{\|x_{L,k} - x_{true}\|}{\|x_{true}\|},$$

under the condition (3.20), it follows from the fact

$$\frac{\|x_{L,k}\|}{\|x_{true}\|} = O(1)$$

(3.23)
and the proof of Theorem 3.6 that (3.21) and (3.22) also hold when the index $k_0$ is replaced by $k = 1, 2, \ldots, k_0$ and a few $k > k_0$. We remark that the estimate (3.23) holds because $\|x_{L,k}\|$ exhibits increasing tendency, and it first approximates $\|x_{true}\|$ from below for $k = 1, 2, \ldots, k_0$ and then starts to deviate from $\|x_{true}\|$ but not too much for a few $k > k_0$. Therefore, we have proved the following theorem.

**Theorem 3.7.** If $L$ is well conditioned and

$$O(tol) < \frac{\|e\|}{\|b_{true}\|},$$

then for $k = 1, 2, \ldots, k_0$ and a few $k > k_0$ we have

$$\|x_{L,k} - x_{true}\| - O(tol) \leq \frac{\|\bar{x}_{L,k} - x_{true}\|}{\|x_{true}\|} \leq \frac{\|x_{L,k} - x_{true}\|}{\|x_{true}\|} + O(tol),$$

i.e.,

$$\frac{\|\bar{x}_{L,k} - x_{true}\|}{\|x_{true}\|} = \frac{\|x_{L,k} - x_{true}\|}{\|x_{true}\|},$$

within the error $O(tol)$ with a generic constant in $O(\cdot)$, meaning that the computed $\bar{x}_{L,k}$ has the same as the exact $x_{L,k}$ as an approximation to $x_{true}$.

It is worthwhile to notice that the relative noise level $\frac{\|e\|}{\|b_{true}\|}$ is typically more or less around $10^{-3}$ in applications, three orders bigger than $10^{-6}$. Combining all the above together, we come to conclude that it is generally enough to set $tol = 10^{-6}$ in LSQR at step 3 of Algorithms 4-5. A smaller $tol$ will result in more inner iterations without any gain in the accuracy of $\bar{x}_{L,k}$ as regularized solutions for $k = 1, 2, \ldots, k_0$ and a few $k > k_0$. Moreover, Theorems 3.6-3.7 indicate that $tol = 10^{-6}$ is generally well conservative and larger $tol$ can be used, so that LSQR uses fewer iterations to achieve the convergence and the MTRSVD algorithms are more efficient.

In summary, our conclusion is that a widely varying choice of $tol$ has no effects of regularization of the MTRSVD algorithms, provided that $tol < \frac{\|e\|}{\|b_{true}\|}$ considerably and the regularization matrix $L$ is well conditioned, but it has substantial effects on the efficiency of MTRSVD. In our numerical experiments, we have found that for each test problem with $\frac{\|e\|}{\|b_{true}\|} = 10^{-2}$ and $10^{-3}$ the computed best regularized solutions obtained by MTRSVD have the same accuracy and the convergence curves of MTRSVD are indistinguishable when taking three $tol = 10^{-6}, 10^{-5}$ and $10^{-4}$.

For a given oversampling parameter $q \geq 4$, we need to determine an optimal $k = k_0$ for finding a best possible regularized solution $x_{L,k_0}$ in the MTRSVD algorithms. It is crucial to realize that, just as in the TSVD method, the parameter $k$ plays the role of the regularization parameter in the MTSVD, TGSVD, TRGSVD and MTRSVD methods. From now on, denote by $x_{k}^{reg}$ the regularized solution at step $k$ obtained by each of them. These methods must exhibit semi-convergence [12, 14, 29]: the error $\|L(x_{k}^{reg} - x_{true})\|$ decreases (correspondingly, $\|Lx_{k}^{reg}\|$ steadily increases) with respect to $k$ in the first stage until some step $k = k_0$ and then starts to increases (correspondingly, $\|Lx_{k}^{reg}\|$ starts to increase considerably) after $k > k_0$. Such $k_0$ is exactly an optimal regularization parameter, at which the regularized solution $x_{k_0}^{reg}$ is most accurate and is thus the best possible one obtained by each of these methods.

Given an oversampling parameter $q$, the algorithms of Wei et al. [32] and Xiang and Zou [34] first generate RGSVDs for a certain fixed $k$ and then determine the
optimal Tikhonov regularization parameter \( \lambda_{\text{opt}} \) by GCV \([12, 14]\). In the \( m \geq n \) case, Wei et al. \([32]\) use Algorithm 4.2 in \([11]\) to determine such a \( k \) adaptively until

\[
\|A - QQ^T A\| \leq \bar{\varepsilon}
\]

is satisfied for some small \( \bar{\varepsilon} \). Then they replace \( A \) by the truncated rank-\( k \) approximation to \( A \) obtained from the GSVD of \( \{Q^T A, L\} \) in (1.7) and determine \( \lambda_{\text{opt}} \); see (2.8) in \([32]\). For the \( m \leq n \) case, they reduce the original large (1.7) to a projected problem that replaces \( A \) and \( L \) by \( AQ \) and \( LQ \), respectively, with \( \|A - AQQ^T\| \leq \bar{\varepsilon} \), and then solve it by using the GSVD of \( \{AQ, LQ\} \) and determining an optimal \( \lambda_{\text{opt}} \).

In the numerical experiments, they take a fixed \( \varepsilon = 10^{-2} \) for all the test problems and noise levels. They emphasize that the choice of an optimal tolerance \( \bar{\varepsilon} \) is an open problem. As a matter of fact, the size of \( \bar{\varepsilon} \) is problem and noise level dependent, and it is impossible to presume a fixed and optimal \( \bar{\varepsilon} \) for all problems and noise levels.

A basic fact is that the smaller the noise level, the more dominant SVD (or GSVD) components of \( A \) are needed \([12, 14]\) to form best regularized solutions. This means that the smaller the noise level, the smaller \( \bar{\varepsilon} \) must be.

In practical applications, for the TSVD and MTSVD methods, one can use the GCV parameter-choice method or the L-curve criterion to determine their regularization parameters \( k_0 \) \([12, 14, 16]\). The L-curve criterion is directly applicable to our MTRSVD algorithms: Given an oversampling parameter \( q \), they proceed from \( k = 1 \) onwards, successively increment \( l = k + q \) and expand \( Q \). The algorithms compute a sequence of regularized solutions \( x_k^{\text{reg}} \), and we plot the curve of \( (\|A x_k^{\text{reg}} - b\|, \|L x_k^{\text{reg}}\|) \) in log-log scale, whose corner corresponds to the best regularized solution \( x_k^{\text{reg}} \) with \( k_0 \) the optimal regularization parameter, at which the semi-convergence of our algorithms occurs. In contrast, the GCV parameter-choice method is not directly applicable to our MTRSVD algorithms, and some nontrivial effects are needed to derive corresponding GCV functions. We will consider the GCV parameter-choice method for our MTRSVD algorithms in future work.

In our next numerical experiments, the true solutions \( x_{\text{true}} \)'s to all the test problems are known, so that for a sequence of regularized solutions \( x_k^{\text{reg}} \) the a-priori relative errors \( \|L(x_k^{\text{reg}} - x_{\text{true}})\|/\|Lx_{\text{true}}\| \) can be computed and the regularization parameter \( k_0 \) of semi-convergence is easily identified for each method by plotting the corresponding convergence curve.

4. Numerical examples. In this section, we report numerical experiments to demonstrate that the MTRSVD algorithms can compute regularized solutions as accurately as the standard TGSVD algorithm and at least as accurately as those obtained by the RGSVD algorithms in \([32]\) and \([34]\). We choose some one dimensional examples from Hansen’s regularization toolboxes \([13]\) and a two dimensional problem from \([15]\). We generated the Gaussian noise vectors \( e \) whose entries are normally distributed with mean zero. We denote the relative noise level \( \varepsilon = \|r\|/\|b_{\text{true}}\| \), and use \( \varepsilon = 10^{-2}, 10^{-3} \) in the experiments. To simulate exact arithmetic, the full reorthogonalization is used during the Lanczos bidiagonalization process. Purely for test purposes, we choose \( L = L_1 \) and \( L_3 \) defined by (1.8) and (1.10), respectively. For \( L = L_2 \), we have found that the results and comparisons are very similar to those for \( L = L_1 \), so we omit the reports on \( L = L_2 \).

Recall that \( x_k^{\text{reg}} \) denotes the regularized solution obtained by each of TGSVD, MTRSVD and RGSVD. We use the the relative error

\[
\frac{\|L(x_k^{\text{reg}} - x_{\text{true}})\|}{\|Lx_{\text{true}}\|}
\]
to plot the convergence curve of each method with respect to \( k \). The TRGSVD algorithms in [32] and [34] are denoted by \texttt{weirgsvd} and \texttt{xiangrgsvd}, respectively, we abbreviate the standard TGSVD algorithm as \texttt{tgsvd} and Algorithms 4–5 as \texttt{mtrsvd}.

Here we make some non-essential modifications on the original \texttt{weirgsvd} and \texttt{xiangrgsvd} in order to compare all the algorithms under consideration more directly and insightfully. The original RGSVD algorithms in [32], [34] are the combinations of RGSVD and general-form Tikhonov regularization. We now truncate rank-\((k + q)\) RGSVD and obtain a rank-\(k\) truncated randomized GSVD (TRGSVD), leading to the corresponding TRGSVD algorithms, such a TRGSVD algorithm was mentioned by Xiang and Zou [34]. The original \texttt{weirgsvd} and \texttt{xiangrgsvd} and the current ones are the same in the spirit of \texttt{tgsvd} and the GSVD with Tikhonov regularization [12, 14], and they will generate the best regularized solutions with essentially the same accuracy. In the tables to be presented, we will list the given oversampling parameter \( q \) and the optimal regularization parameter \( k_0 \) in the braces. We use the Matlab function \texttt{lsqr.m} to solve the least squares problems (3.11) with the default stopping tolerance \( tol = 10^{-6} \).

We have observed that for \( \varepsilon = 10^{-2}, 10^{-3} \) the three convergence curves of \texttt{mtrsvd} are indistinguishable for each test problem when taking \( tol = 10^{-6}, 10^{-5}, 10^{-4} \), respectively, and the computed best regularized solutions by \texttt{mtrsvd} for these three \( tol \) have the same accuracy. As a result, for the sake of uniqueness and length, we will only report the results on \( tol = 10^{-6} \).

All the computations are carried out in Matlab R2015b 64-bit on Intel Core i3-2120 CPU 3.30GHz processor and 4 GB RAM.

### 4.1. The \( m \geq n \) case.

We first present the results on four one dimensional test problems from Hansen’s regularization toolbox [13], and then report the results on a two dimensional test problem from Hansen’s regularization toolbox [15].

#### 4.1.1. The one dimensional case.

All test problems arises from the discretization of the first kind Fredholm integral equations

\[
\int_a^b k(s, t)x(t)dt = f(s), \quad c \leq s \leq d.
\]

For each problem we use the code of [13] to generate \( A \), the true solution \( x_{true} \) and noise-free right-hand side \( b_{true} \). The four test problems are severely, moderately and mildly ill-posed, respectively; see Table 1, where we choose the parameter “example = 2” for the test problem deriv2.

| Problem | Description | Ill-posedness |
|---------|-------------|---------------|
| shaw    | One dimensional image restoration model | severe |
| gravity | One dimensional gravity surveying problem | severe |
| heat    | Inverse heat equation | moderate |
| deriv2  | Computation of second derivative | mild |

In Table 2, we display the relative errors of the best regularized solutions \( x_{k_0}^{reg} \) by \texttt{tgsvd}, \texttt{weirgsvd} and \texttt{mtrsvd} with \( L = L_1 \) and \( \varepsilon = 10^{-2}, 10^{-3} \), respectively. They illustrate that for all test problems with \( m = n = 1,024 \) the solution accuracy of \texttt{mtrsvd} is very comparable to that of \texttt{tgsvd} and \texttt{weirgsvd}. For \( m = n = 10,240 \), \texttt{tgsvd} and \texttt{weirgsvd} are out of memory in our computer, but \texttt{mtrsvd} works well and the best
The comparison of Algorithm 4 (mtrsvd) and the others with \( L = L_1 \) and \( \epsilon = 10^{-2}, 10^{-3} \).

| \( \epsilon = 10^{-2} \) | \( m = n = 1,024 \) | \( m = n = 10,240 \) |
|------------------------|-----------------|-----------------|
| \( q \) | \( q \) | \( mtrsvd \) | \( weirgsvd \) | \( mtrsvd \) | \( weirgsvd \) | \( mtrsvd \) |
| \( mtrsvd \) | \( weirgsvd \) | \( mtrsvd \) |
| shaw | 9 | 0.2043(6) | 0.2043(7) | 0.2043(6) | 0.1946(7) |
| gravity | 11 | 0.3205(7) | 0.3203(8) | 0.3202(8) | 0.2594(9) |
| heat | 7 | 0.2526(23) | 0.2544(23) | 0.2457(23) | 0.2285(23) |
| deriv2 | 11 | 0.4264(5) | 0.4324(6) | 0.4411(6) | 0.3621(16) |

\( \epsilon = 10^{-3} \)

| \( m = n = 1,024 \) | \( m = n = 10,240 \) |
|-----------------|-----------------|
| \( q \) | \( q \) | \( mtrsvd \) | \( weirgsvd \) | \( mtrsvd \) | \( weirgsvd \) | \( mtrsvd \) |
| \( mtrsvd \) | \( weirgsvd \) | \( mtrsvd \) |
| shaw | 9 | 0.1681(8) | 0.1681(9) | 0.1681(9) | 0.1428(9) |
| gravity | 7 | 0.2660(10) | 0.2675(11) | 0.2660(11) | 0.2532(11) |
| heat | 8 | 0.1664(30) | 0.1673(31) | 0.1623(29) | 0.1399(36) |
| deriv2 | 6 | 0.3341(11) | 0.3360(12) | 0.3462(12) | 0.2916(12) |

A regularized solution is more accurate than the corresponding one for \( m = n = 1,024 \). We observe from the table that for each test problem the best regularized solution by each algorithm is correspondingly more accurate for \( \epsilon = 10^{-3} \) than \( \epsilon = 10^{-2} \); for each algorithm, the optimal regularization parameter \( k_0 \) is bigger for \( \epsilon = 10^{-3} \) than for \( \epsilon = 10^{-2} \). All these are expected and justify that the smaller the noise level \( \epsilon \) is, the more SVD (or GSVD) dominant components of \( A \) or \( \{A, L\} \) are needed to form best regularized solutions. Finally, as is seen, for each problem and the given \( \epsilon \), the optimal \( k_0 \) are almost the same for all the algorithms. This indicates that mtrsvd and weirgsvd effectively capture the dominant SVD and GSVD components of \( A \) and \( \{A, L\} \), respectively.

In Table 3, we display the relative errors of the best regularized solutions by tgsvd, weirgsvd and mtrsvd with \( L = L_3 \) and \( \epsilon = 10^{-2}, 10^{-3} \), respectively. The results and performance evaluations on the three algorithms are analogous to those for \( L = L_1 \), and the details are thus omitted.

Figure 1 depicts the convergence processes of mtrsvd, tgsvd and weirgsvd as \( k \) increases for the four test problems with \( L = L_3 \), \( \epsilon = 10^{-3} \) and \( m = n = 1,024 \). We can see that the three algorithms have very similar convergence processes and the relative errors of regularized solutions obtained by mtrsvd are almost identical to those by tgsvd and weirgsvd as \( k \) increases until the occurrence of semi-convergence. For the other problems, we have observed similar phenomena. These indicate that the three algorithms have the same or highly competitive regularizing effects.

Figure 2 depicts the number of inner iterations used by LSQR versus the parameter \( k \). We clearly observe that the number of inner iterations exhibits a considerable decreasing tendency as \( k \) increases for the chosen test problems with \( L = L_3 \), \( \epsilon = 10^{-3} \) and \( m = n = 1,024 \). LSQR becomes substantially more efficient with \( k \) increasing. For \( L = L_1 \), we have similar findings. A distinction is that, for each problem, LSQR uses fewer inner iterations to converge for \( L_1 \) than for \( L_3 \).
Fig. 1. The semi-convergence processes of mtrsvd, tgsvd and weirgsvd for the four test problems with $L = L_3$, $\varepsilon = 10^{-3}$ and $m = n = 1,024$: (a) shaw; (b) gravity; (c) heat; (d) deriv2.

Fig. 2. The numbers of inner iterations versus $k$ for Algorithm 4 (mtrsvd) with $L = L_3$, $\varepsilon = 10^{-3}$ and $m = n = 1,024$: (a) shaw; (b) gravity; (c) heat; (d) deriv2.
Table 3
The comparison of Algorithm 4 (mtrsvd) and the others with $L = L_3$ and $\varepsilon = 10^{-2}$, $10^{-3}$.

| $\varepsilon = 10^{-2}$ | $m = n = 1,024$ | $m = n = 10,240$ |
|--------------------------|-----------------|-------------------|
| $q$ | tgsvd | weirgsvd | mtrsvd | weirgsvd | mtrsvd | weirgsvd | mtrsvd |
| shaw | 11 | 0.2030(7) | 0.2030(8) | 0.2024(8) | - | 0.1984(7) |
| gravity | 10 | 0.3340(8) | 0.3342(8) | 0.3339(8) | - | 0.2292(9) |
| heat | 7 | 0.2966(23) | 0.2856(23) | 0.2695(22) | - | 0.2386(23) |
| deriv2 | 9 | 0.4365(6) | 0.4446(6) | 0.4430(7) | - | 0.4207(10) |

| $\varepsilon = 10^{-3}$ | $m = n = 1,024$ | $m = n = 10,240$ |
|--------------------------|-----------------|-------------------|
| $q$ | tgsvd | weirgsvd | mtrsvd | weirgsvd | mtrsvd | weirgsvd | mtrsvd |
| shaw | 4 | 0.1694(8) | 0.1694(8) | 0.1694(8) | - | 0.1431(9) |
| gravity | 8 | 0.2838(10) | 0.2830(10) | 0.2811(10) | - | 0.1789(9) |
| heat | 12 | 0.1626(30) | 0.1616(30) | 0.1610(30) | - | 0.1468(35) |
| deriv2 | 8 | 0.3465(10) | 0.3499(10) | 0.3550(10) | - | 0.3129(13) |

4.1.2. The two dimensional case. In this subsection, we test the problem seismicwavetomo which is from [15] and creates a two dimensional seismic tomography. We use the code of [15] to generate an $ps \times n^2$ coefficient matrix $A$, the true solution $x_{true}$ and noise-free right-hand side $b_{true}$. We take $N = 32$ and 100 with default $s = N$ and $p = 2N$, respectively, that is, we generate $A \in \mathbb{R}^{2,048 \times 1,024}$ and $A \in \mathbb{R}^{20,000 \times 10,000}$.

Table 4
The relative errors for seismicwavetomo.

| $\varepsilon$ | $q$ | $L = L_1$ | $L = L_3$ |
|---------------|-----|-----------|-----------|
| $m = 2,048$ and $n = 1,024$ | | | |
| $10^{-2}$ | 70 | 0.6397(347) | 0.6358(323) | 0.6116(305) | 0.7526(369) | 0.7498(380) | 0.7181(285) |
| $10^{-3}$ | 42 | 0.3117(658) | 0.3083(603) | 0.2982(586) | 0.3777(623) | 0.3691(633) | 0.3451(604) |
| $m = 20,000$ and $n = 10,000$ | | | |
| $10^{-2}$ | 141 | 0.8691(419) | 0.8691(419) | 295 | 0.9092(345) |
| $10^{-3}$ | 951 | 0.7766(1249) | 0.7766(1249) | 53 | 0.8949(1147) |

Table 4 shows the relative errors of the best regularized solutions obtained by mtrsvd, tgsvd and weirgsvd with $L = L_1, L_3$ and $\varepsilon = 10^{-2}, 10^{-3}$, respectively, where tgsvd and weirgsvd are out of memory for $m = 20,000, n = 10,000$. Obviously, the relative errors of the best regularized solutions by mtrsvd are at least as accurate as those by tgsvd and weirgsvd for the two given $\varepsilon$ and $m = 2,048, n = 1,024$, and mtrsvd is more practical than tgsvd and weirgsvd for large scale problems.

We next investigate how mtrsvd behaves as the oversampling parameter $q$ varies.
Table 5

The relative errors for seismicwavetomo of $m = 20,000, n = 10,000$.

| $q$ | $mtrsvd$ | $q$ | $mtrsvd$ |
|-----|---------|-----|---------|
| 75  | 0.9489(405) | 10  | 0.7907(1110) |
| 173 | 0.9483(407) | 587 | 0.7802(1213) |
| 176 | 0.9475(424) | 951 | 0.7766(1249) |

Fig. 3. The relative errors of $tgsvd$, $weirgsvd$ and $mtrsvd$, and inner iterations versus $k$ of Algorithm 4 ($mtrsvd$) for the problem seismicwavetomo of $m = 2,048, n = 1,024$ with $L = L_3$ and $\varepsilon = 10^{-3}$.

for this problem with $m = 20,000$ and $n = 10,000$. Table 5 shows the relative errors of the best regularized solutions obtained by $mtrsvd$ for varying $q$ with $L = L_1, L_3$ and $\varepsilon = 10^{-2}, 10^{-3}$, respectively. As we can see, the relative errors of the best regularized solutions by $mtrsvd$ for seismicwavetomo decrease a little bit with $q$ increasing. This confirms our theory that bigger $q$ should generally generate more accurate rank-$k$ approximation to $A$, so that the regularized solutions could be more accurate.

Figures 3 draws the convergence processes of $mtrsvd$ $tgsvd$ and $weirgsvd$ for $m = 20,48, n = 10,24$ and the inner iterations versus the parameter $k$ with $\varepsilon = 10^{-3}$ and $L = L_3$. We can see that the best regularized solution by $mtrsvd$ is more accurate than the counterparts by $tgsvd$ and $weirgsvd$ and LSQR uses substantially fewer iterations as $k$ increases. Compared with the results on the one dimensional problems, however, we observe a remarkable difference that the optimal regularization parameter $k_0$ now becomes much bigger. The reason is that for this problem, as we have numerically justified by plotting the discrete Picard condition, the Fourier coefficients $|u_i^T b_{true}|$ do not decay considerably faster than the generalized singular values $\sigma_i$ of $\{A, L, \}$, where the $u_i$ are the first $\min(p,n)$ left singular vectors of $\{A, L\}$. Recall that the GSVD of $\{A, L\}$ is $A = UCZ^{-1}$ and $L = VSZ^{-1}$, where $C \in \mathbb{R}^{m \times n}$ and $S \in \mathbb{R}^{p \times n}$ are diagonal matrices with the diagonal entries $c_i$ and $s_i$, respectively, $CTC + S^TS = I$, $\sigma_i = c_i/s_i$, $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{p \times p}$ are orthogonal, and the columns $u_i$ of $U$ are called the left singular vectors. This means that a good regularized solution must include many dominant GSVD components of $\{A, L\}$.

4.2. The $m \leq n$ case. We now test Algorithm 5 ($mtrsvd$), $tgsvd$, $weirgsvd$ and $xiangrgsvd$ on the test problems in Table 1. In Table 6, we display the relative errors of the best regularized solutions obtained by $mtrsvd$, $tgsvd$, $weirgsvd$ and $xiangrgsvd$ with $L = L_1$ and $\varepsilon = 10^{-2}, 10^{-3}$, respectively.
Table 6
The comparison of Algorithm 5 (mtrsvd) and the others with $L = L_1$ and $\varepsilon = 10^{-2}$, $10^{-3}$.

| $\varepsilon = 10^{-2}$         | $m = n = 1,024$ | $m = n = 10,240$ |
|--------------------------------|----------------|-----------------|
| $q$   | tgsvd | xiangrssvd | weirgsvd | mtrsvd | xiangrssvd | mtrsvd |
| shaw | 11    | 0.2099(6) | 0.2099(7) | 0.2099(7) | 0.2097(7) | 0.1666(8) | 0.1669(8) |
| gravity | 9   | 0.3004(8) | 0.2993(9) | 0.2993(9) | 0.2993(9) | 0.2743(10) | 0.2785(10) |
| heat | 7    | 0.2228(27) | 0.3561(23) | 0.3561(23) | 0.2488(24) | 0.3535(23) | 0.2369(25) |
| deriv2 | 12   | 0.4329(5) | 3.1031(1)  | 3.1031(1)  | 0.4455(6)  | 3.1025(1)  | 0.4343(8)  |

| $\varepsilon = 10^{-3}$         | $m = n = 1,024$ | $m = n = 10,240$ |
|--------------------------------|----------------|-----------------|
| $q$   | tgsvd | xiangrssvd | weirgsvd | mtrsvd | xiangrssvd | mtrsvd |
| shaw | 6    | 0.1946(6) | 0.1967(7) | 0.1967(7) | 0.1942(7) | 0.1353(9) | 0.1311(9) |
| gravity | 6  | 0.2556(12) | 0.2382(12) | 0.2382(12) | 0.2577(11) | 0.2443(12) | 0.2223(12) |
| heat | 8    | 0.1543(30) | 0.1714(30) | 0.1714(30) | 0.1564(29) | 0.1801(32) | 0.1523(32) |
| deriv2 | 6   | 0.3342(12) | 3.0987(1)  | 3.0987(1)  | 0.3790(8)  | 3.0985(1)  | 0.3815(8)  |

The results indicate that for $m = n = 1,024$ mtrsvd computes the best regularized solution with very similar accuracy to those by tgsvd and weirgsvd, xiangrssvd for severely and moderately ill-posed problems, but the solution accuracy by mtrsvd is much higher than that by xiangrssvd and weirgsvd for the mildly ill-posed problem deriv2. Actually, the best regularized solutions by xiangrssvd and weirgsvd have no accuracy since their relative errors are over 300%! As is expected, whenever an algorithm has regularizing effects and can compute a regularized solution with some accuracy, the smaller $\varepsilon$ is, the bigger $k_0$ is and the more accurate regularized solution is, except for shaw of $m = 1,024$ and $n = 1,024$ where the $k_0$ are the same for each algorithm with $\varepsilon = 10^{-2}, 10^{-3}$.

Mathematically, weirgsvd is the same as xiangrssvd. Table 6 confirms that these two algorithms compute the same regularized solutions for $m = n = 1,024$. For this reason, we only report the results obtained by xiangrssvd for $m = n = 10,240$. Still, xiangrssvd fails to solve deriv2 and the relative errors of the best regularized solutions are over 300%, but mtrsvd is successful to obtain good regularized solutions.

In Table 7, we display the relative errors of best regularized solutions by all the algorithms with $L = L_3$ and $\varepsilon = 10^{-2}, 10^{-3}$, respectively. Clearly, we can observe very similar phenomena to those in Table 6.

Figure 4 depicts the curves of convergence processes of all the algorithms for the four test problems shaw, gravity, heat and deriv2 with $L = L_3$, $\varepsilon = 10^{-3}$ and $m = n = 1,024$. Figure 5 does the same job for these four problems with $L = L_3$, $\varepsilon = 10^{-3}$ and $m = n = 10,240$. From the two figures, we can see that for the severely ill-posed problem shaw and gravity, the relative errors obtained by mtrsvd are almost identical to those by tgsvd and weirgsvd, xiangrssvd. For the moderately and mildly ill-posed problems, mtrsvd also behaves like tgsvd, but the best regularized solutions obtained by weirgsvd and xiangrssvd for the mildly ill-posed problem deriv2 have no accuracy and their relative errors are over 300%. Also, we notice that for the moderately ill-posed problem heat with $L = L_3$, the best regularized solutions by weirgsvd and xiangrssvd are much less accurate than those by tgsvd and mtrsvd.
Fig. 4. The relative errors of Algorithm 5 (mtrsvd) with $L = L_3$ and $\varepsilon = 10^{-3}$ and $m = n = 1,024$: (a) shaw; (b) gravity; (c) heat; (d) deriv2.

Fig. 5. The relative errors of Algorithm 5 (mtrsvd) with $L = L_3$ and $\varepsilon = 10^{-3}$ and $m = n = 10,240$: (a) shaw; (b) gravity; (c) heat; (d) deriv2.
Table 7
The comparison of Algorithm 5 (mtrsvd) and the others with $L = L_3$ and $\varepsilon = 10^{-2}, 10^{-3}$.

| $\varepsilon = 10^{-2}$ |  |  |  |  |  |  |
|-------------------------|-------------------|------------------|-------------------|-------------------|-------------------|
| $m = n = 1,024$         | $m = n = 10,240$  |  |  |  |  |
| $q$         | tgsvd | xiangrsvd | weirgsvd | mtrsvd | xiangrsvd | mtrsvd |
| shaw        | 0.2000(7) | 0.2000(7) | 0.2000(7) | 0.1993(7) | 0.1475(9) | 0.1371(9) |
| gravity     | 0.3287(8) | 0.3265(8) | 0.3265(8) | 0.3280(8) | 0.2315(12) | 0.1787(12) |
| heat        | 0.3065(24) | 0.3721(20) | 0.3721(20) | 0.3268(21) | 0.1806(35) | 0.1402(35) |
| deriv2      | 0.4481(6) | 3.1009(1) | 3.1009(1) | 0.4905(5) | 3.0993(1) | 0.3758(9) |
| $\varepsilon = 10^{-3}$ |  |  |  |  |  |  |
| $m = n = 1,024$         | $m = n = 10,240$  |  |  |  |  |
| $q$         | tgsvd | xiangrsvd | weirgsvd | mtrsvd | xiangrsvd | mtrsvd |
| shaw        | 0.1659(8) | 0.1662(8) | 0.1662(8) | 0.1659(8) | 0.2010(7) | 0.1998(7) |
| gravity     | 0.2686(10) | 0.2655(10) | 0.2655(10) | 0.2668(10) | 0.2891(11) | 0.2926(11) |
| heat        | 0.1689(31) | 0.2851(30) | 0.2851(30) | 0.1825(28) | 0.4519(21) | 0.3371(22) |
| deriv2      | 0.3374(12) | 3.0999(1) | 3.0999(1) | 0.3891(8) | 3.0984(1) | 0.3857(10) |

Finally, we observe from Figure 6 that the number of the inner iterations used by LSQR decrease as $k$ increases for some chosen test problems when $L = L_3$, $\varepsilon = 10^{-3}$ and $m = n = 1,024$. We see that after a few iterations, LSQR only needs two or three hundreds iterations and even no more than one hundred iterations to achieve the prescribed tolerance.

5. Conclusion. In this paper, we have proposed two MTRSVD algorithms for solving the overdetermined and underdetermined (1.1) with general-form regularization, respectively. We have established a number of sharp error bounds for the approximation accuracy of randomized approximate SVDs for three kinds of ill-posed problems and their truncated rank-$k$ ones. These results have improved the existing bounds substantially and provided strong theoretical supports for the effectiveness of randomized algorithms for solving ill-posed problems. We have considered the conditioning of inner least squares problems and shown that it becomes better conditioned as the regularization parameter $k$ increases. As a consequence, LSQR generally converge faster with $k$ and uses fewer iterations to achieve the prescribed tolerance, which has been confirmed numerically. In the meantime, we have given a detailed analysis on the stopping tolerance of LSQR for inner least squares problems and shown how to choose it in order to guarantee that the computed regularized solutions have the same accuracy as the ones when the problems are solved exactly. Numerical experiments have confirmed our theory.

A practical advantage of MTRSVD is its applicability to truly large scale problems for both overdetermined and underdetermined ill-posed problems, while TGSVD suits only for small to medium scale problems. For the overdetermined problems, the TRGSVD algorithm in [32], though theoretically good, are practically infeasible since it required to compute the GSVD of the large matrix pair $\{B, L\}$ with $B = Q^T A \in \mathbb{R}^{l \times n}$ and invert a large $n \times n$ matrix to get the right singular vector matrix; for the underdetermined problems, the TRGSVD algorithms in [32, 34] seems to lack necessary theoretical supports and may not work well. Some of our numerical
experiments have confirmed this deficiency.

Numerical experiments have demonstrated that our MTRSVD algorithms can compute regularized solutions with very similar accuracy to those by the standard TGSVD algorithm and they are at least as effective as the TRGSVD algorithms in [32, 34] for solving both overdetermined and underdetermined (1.1).

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REFERENCES

[1] R. C. Aster, B. Borchers, and C. H. Thurber, Parameter Estimation and Inverse Problems, Second Edition, Elsevier, New York, 2013.
[2] Å. Björck, Numerical Methods for Least Squares Problems, SIAM, Philadelphia, PA, 1996.
[3] J. J. M. Cuppen, Calculating the isochromes of ventricular depolarization, SIAM J. Sci. Statist. Comput., 5 (1984), pp. 105–120.
[4] M. G. Cox, Data approximation by splines in one and two independent variables, in A. Iserles and M. J. D. Powell (Eds.), The State of the Art in Numerical Analysis, Clarendon Press, Oxford, UK, 1987, pp. 111–138.
[5] L. Eldén, A weighted pseudoinverse, generalized singular values and constrained least squares problems, BIT, 22 (1982), pp. 487–502.
[6] H. W. Engl, Regularization methods for the stable solution of inverse problems, Surveys Math. Indus., 3 (1993), pp. 71–143.
[7] H. W. Engl, M. Hanke, and A. Neubauer, Regularization of Inverse Problems, Kluwer Academic Publishers, 2000.
[8] G. H. Golub and C. F. Van Loan, Matrix Computations, 4th ed., Johns Hopkins University Press, Baltimore, MD, 2013.
[9] M. Gu, Subspace iteration randomization and singular value problems, SIAM J. Sci. Comput., 37 (2015), pp. A1139–A1173.

[10] Y. Gu, W. J. Yu, and Y. H. Li, Efficient randomized algorithms for adaptive low-rank factorizations of large matrices, arXiv:1606.09402, 2016.

[11] N. Halko, P. G. Martinsson, and J. A. Tropp, Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions, SIAM Rev., 53 (2011), pp. 217–288.

[12] P. C. Hansen, Rank-Deficient and Discrete Ill-Posed Problems: Numerical Aspects of Linear Inversion, SIAM, Philadelphia, PA, 1998.

[13] ———, Regularization tools version 4.0 for Matlab 7.3, Numer. Algor., 46 (2007), pp. 189–194.

[14] ———, Discrete Inverse Problems: Insight and Algorithms, SIAM, Philadelphia, PA, 2010.

[15] P. C. Hansen, M. Saxild-Hansen, AIR tools—a MATLAB package of algebraic iterative reconstruction methods, J. Comput. Appl. Math., 236 (2012), pp. 2167–2178.

[16] P. C. Hansen, T. Sekii, and H. Shihahashi, The modified truncated SVD method for regularization in general form, SIAM J. Sci. Comput., 13 (1992), pp. 1142–1150.

[17] N. J. Higham, Accuracy and Stability of Numerical Algorithms, 2nd ed., SIAM, Philadelphia, PA, 2002.

[18] B. Hofmann, Regularization for Applied Inverse and Ill-posed Problems, Teubner, Stuttgart, Germany, 1986.

[19] Z. Jia, The regularization theory of the Krylov iterative solvers LSQR, CGLS, LSMR and CGME For linear discrete ill-posed problems, arXiv:math.NA/1608.05907, 2016.

[20] ———, The regularization theory of the Krylov iterative solvers LSQR and CGLS for linear discrete ill-posed problems, Part I: the simple singular value case, arXiv: math.NA/1701.05708, 2017.

[21] ———, Regularizing effects of the Krylov iterative solvers CGME and LSMR for linear discrete ill-posed problems with an application to truncated randomized SVDs, (2017), manuscript.

[22] J. Kaipio and E. Somersalo, Statistical and Computational Inverse Problems, Applied Mathematical Sciences 160, Springer, 2005.

[23] M. E. Kilmer, P. C. Hansen, and M. I. Espanol, A projection-based approach to general-form Tikhonov regularization, SIAM J. Sci. Comput., 29 (2007), pp. 315–339.

[24] E. Liberty, F. Woolfe, P.-G. Martinsson, V. Rokhlin, and M. Tygert, Randomized algorithms for the low-rank approximation of matrices, Proc. Natl. Acad. Sci. USA, 104 (2007), pp. 20167–20172.

[25] K. Miller, Least squares methods for ill-posed problems with a prescribed bound, SIAM J. Math. Anal., 1 (1970), pp. 52–74.

[26] J. L. Mueller and S. Siltanen, Linear and Nonlinear Inverse Problems with Practical Applications, SIAM, Philadelphia, PA, 2012.

[27] P.-G. Martinsson, V. Rokhlin, and M. Tygert, A randomized algorithm for the decomposition of matrices, Appl. Comput. Harmon. Anal., 30 (2011), pp. 47–68.

[28] X. Meng, M. A. Saunders, and M. W. Maroney, LSRN: A parallel iterative solver for strongly over- or underdetermined systems, SIAM J. Sci. Comput., 36 (2014), pp. C95–C118.

[29] F. Natterer, The Mathematics of Computerized Tomography, John Wiley, New York, 1986.

[30] C. C. Paige and M. A. Saunders, LSQR: An algorithm for sparse linear equations and sparse least squares, ACM Trans. Math. Soft., 8 (1982), pp. 43–71.

[31] V. Rokhlin, A. Szlam, and M. Tygert, A randomized algorithm for principal component analysis, SIAM J. Matrix Anal. Appl., 31 (2009), pp. 1100–1124.

[32] Y. Wei, P. P. Xie, and L. P. Zhang, Tikhonov regularization and randomized GSVD, SIAM J. Matrix Anal. Appl., 37 (2016), pp. 649–675.

[33] H. Xiang and J. Zou, Regularization with randomized SVD for large-scale discrete inverse problems, Inverse Probl., 29 (2013), 085008.

[34] ———, Randomized algorithms for large-scale inverse problems with general Tikhonov regularizations, Inverse Probl., 31 (2015), 085008.