Regularization properties of Krylov iterative solvers
CGME and LSMR for linear discrete ill-posed problems
with an application to truncated randomized SVDs

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Abstract
For the large-scale linear discrete ill-posed problem \( \min \| Ax - b \| \) or \( Ax = b \) with \( b \) contaminated by Gaussian white noise, the following Krylov solvers are commonly used: LSQR, and its mathematically equivalent CGLS (i.e., the Conjugate Gradient (CG) method applied to \( A^T Ax = A^T b \)), CGME (i.e., the CG method applied to \( \min \| A^T y - b \| \) or \( A^T y = b \) with \( x = A^T y \)), and LSMR (i.e., the minimal residual (MINRES) method applied to \( A^T Ax = A^T b \)). These methods have intrinsic regularizing effects, where the number \( k \) of iterations plays the role of the regularization parameter. In this paper, we analyze the regularizing effects of CGME and LSMR and establish a number of results including the filtered SVD expansion of CGME iterates, which prove that the 2-norm filtering best possible regularized solutions by CGME and LSMR are less accurate than and at least as accurate as those by LSQR, respectively. We also prove that the semi-convergence of CGME and LSMR always occurs no later and sooner than that of LSQR, respectively. As a byproduct, using the analysis approach for CGME, we improve a fundamental result on the accuracy of the truncated rank \( k \) approximate SVD of \( A \) generated by randomized algorithms, and reveal how the truncation step damages the accuracy. Numerical experiments justify our results on CGME and LSMR.

Keywords Discrete ill-posed · Rank \( k \) approximations · TSVD solution · Semi-convergence · Regularized solution · Regularizing effects · CGME · LSMR · LSQR

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1 Introduction and preliminaries

Consider the linear discrete ill-posed problem

$$\min_{x \in \mathbb{R}^n} \|Ax - b\| \text{ or } Ax = b, \quad A \in \mathbb{R}^{m \times n}, \ b \in \mathbb{R}^m, \quad (1.1)$$

where the norm $\| \cdot \|$ is the 2-norm of a vector or matrix, and $A$ is extremely ill-conditioned with its singular values decaying to zero without a noticeable gap. We simply assume that $m \geq n$ since the results in this paper hold for both the $m \geq n$ and $m \leq n$ cases. Problem (1.1) arises from many applications, typically from the discretization of the first kind Fredholm integral equation

$$Kx = (Kx)(s) = \int_{\Omega} k(s, t)x(t)dt = g(s) = g, \ s \in \Omega \subset \mathbb{R}^q, \quad (1.2)$$

where the kernel $k(s, t) \in L^2(\Omega \times \Omega)$ and $g(s)$ are known functions, while $x(t)$ is the unknown function to be sought. Applications include image deblurring, signal processing, geophysics, computerized tomography, heat propagation, biomedical and optical imaging, and groundwater modeling; see, e.g., [1, 9, 10, 24, 35–37, 39, 45].

The right-hand side $b = b_{true} + e$ is assumed to be contaminated by a Gaussian white noise $e$, caused by measurement, modeling or discretization errors, where $b_{true}$ is noise-free and $\|e\| < \|b_{true}\|$. Because of the presence of noise $e$ and the extreme ill-conditioning of $A$, the naive solution $x_{naive} = A^+b$ of (1.1) generally bears no relation to the true solution $x_{true} = A^+b_{true}$, where $^+$ denotes the Moore-Penrose inverse of a matrix. Therefore, one has to use regularization to extract a best possible approximation to $x_{true}$.

For a Gaussian white noise $e$, throughout the paper, we always assume that $b_{true}$ satisfies the discrete Picard condition $\|A^+b_{true}\| \leq C$ with some constant $C$ for $\|A^+\|$ arbitrarily large [1, 13, 20–22, 24, 36]. Without loss of generality, assume that $Ax_{true} = b_{true}$. Then a dominating regularization approach is to solve the problem

$$\min_{x \in \mathbb{R}^n} \|Lx\| \text{ subject to } \|Ax - b\| \leq \tau \|e\| \quad (1.3)$$

with $\tau > 1$ slightly [22, 24], where $L$ is a regularization matrix and its suitable choice is based on a-prior information on $x_{true}$.

If $L \neq I$, problem (1.3), in principle, can be transformed into the standard-form problem (1.3) [22, 24], which is a 2-norm filtering regularization problem. Without loss of generality, we are concerned with $L = I$ in this paper. Let

$$A = U \left( \begin{array}{c} \Sigma \\ 0 \end{array} \right) V^T \quad (1.4)$$

be the singular value decomposition (SVD), where $U = (u_1, u_2, \ldots, u_m) \in \mathbb{R}^{m \times m}$ and $V = (v_1, v_2, \ldots, v_n) \in \mathbb{R}^{n \times n}$ are orthogonal, $\Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n) \in \mathbb{R}^{n \times n}$ with the singular values $\sigma_1 > \sigma_2 > \cdots > \sigma_n > 0$ assumed to be simple, the superscript $T$ denotes the transpose of a matrix or vector.

The truncated SVD (TSVD) method [20, 22, 24] is a reliable and commonly used method for solving small to modest sized (1.3), and it solves

$$\min \|x\| \text{ subject to } \|A_kx - b\| = \text{min} \quad (1.5)$$
for some $k$, where $A_k = U_k \Sigma_k V_k^T$ is a best rank $k$ approximation to $A$ with respect to the 2-norm with $U_k = (u_1, \ldots, u_k)$, $V_k = (v_1, \ldots, v_k)$ and $\Sigma_k = \text{diag}(\sigma_1, \ldots, \sigma_k)$; it holds that $\|A - A_k\| = \sigma_{k+1}$ [3, p.12], and $x_{k0}^{TSVD} = A_k^+b$ solves (1.5), called the TSVD regularized solution. For the Gaussian white noise $e$ with the expected values $E(|u_i^T e|) = \eta$, $i = 1, 2, \ldots, m$, the optimal regularization parameter $k_0$, called the transition point, is the index that satisfies

$$|u_{k0}^T b| \approx |u_{k0}^T b_{true}| > |u_{k0+1}^T e| \approx \eta, \ |u_{k0+1}^T b| \approx |u_{k0+1}^T e| \approx \eta; \quad (1.6)$$

see [24, p.42, 98] and [22, p.70–1]. It has been justified that $x_{k0}^{TSVD}$ is essentially a 2-norm filtering best possible solution of (1.3); see [44], [21], [22, p.109–11] and [24, Sections 4.2 and 4.4]. As a result, we can take $x_{k0}^{TSVD}$ as the standard reference when assessing the regularization ability of a 2-norm filtering regularization method.

Krylov iterative solvers have been widely used for solving a large (1.1); see, e.g., [1, 10, 14, 17, 22, 24, 37]. Specifically, the CGLS method [15, 27] and its mathematically equivalent LSQR method [41], the CGME method [3, 4, 6, 17, 18] and the LSMR method [4, 5, 11] have been commonly used for solving a large (1.1). These methods are deterministic 2-norm filtering regularization methods and have been intensively studied [1, 8, 14, 17, 18, 22, 24, 28, 29], and they have general regularizing effects and exhibit semi-convergence [39, p.89]; see also [3, p.314], [4, p.733], [22, p.135], and [24, p.110].

The behavior of ill-posed problems depends on the decay rate of $\sigma_j$. Hoffmann [30] has characterized the degree of ill-posedness of (1.1) as follows: If $\sigma_j = \mathcal{O}(\rho^{-j})$ with $\rho > 1$, $j = 1, 2, \ldots, n$, then (1.1) is severely ill-posed; if $\sigma_j = \mathcal{O}(j^{-\alpha})$, then (1.1) is mildly or moderately ill-posed for $\frac{1}{2} < \alpha \leq 1$ or $\alpha > 1$. This definition has been widely used [1, 10, 22, 24] and supplemented in [31, 32].

It has long been known (cf. [19, 22–24]) that if the singular values of the projection matrices involved in LSQR, called the Ritz values, approximate the first large singular values in natural order then the regularizing effects of LSQR are as good as those of the TSVD method and the two methods can compute 2-norm filtering best possible regularized solutions with the same accuracy. As we will see clearly, the same results hold for CGME and LSMR when the singular values of projection matrices approximate the large singular values of $A$ and $A^TA$ in natural order, respectively.

If a 2-norm filtering regularized solution of (1.1) is as accurate as $x_{k0}^{TSVD}$, it is called a 2-norm filtering best possible regularized solution. If the 2-norm filtering regularized solution by a regularization method at semi-convergence is such a best possible one, then the solver is said to have the full regularization. Otherwise, the solver has only the partial regularization. This definition is introduced in [31, 32].

The analysis on the TSVD method and the Tikhonov regularization method [22, 24] shows that the regularizing effects of a regularization method depend on its ability to acquire the $k_0$ dominant SVD components of $A$ and meanwhile suppress the SVD components associated with the $n - k_0$ small singular values. Notice that CGME, LSMR, and LSQR compute approximations from the same $k$-dimensional subspace, and they are based on the same Golub-Kahan bidiagonalization process that combines the information from the original data in an adaptively optimal way. Therefore, for these three solvers, if a rank $k$ approximation to $A$ or $A^TA$ is more accurate and
its $k$ non-zero singular values better approximate some of the $k_0$ large singular values of $A$ or $A^T A$, the method will have better regularization ability, so that the best regularized solution obtained by it is more accurate.

For the cases that $\sigma_i$ are simple, the author [32, 33] has proved that, for LSQR, the $k$ Ritz values converge to the $k$ large singular values of $A$ in natural order and Golub-Kahan bidiagonalization always generates a near best rank $k$ approximation until $k = k_0$ for the severely and moderately ill-posed problems with suitable $\rho > 1$ and $\alpha > 1$, meaning that LSQR and CGLS have the full regularization. For the singular value models $\sigma_i = \rho^{-i}$ and $\sigma_i = i^{-\alpha}$, it is sufficient for $\rho = 1 + \sqrt{62}$ and $\alpha$ to be reasonably bigger than one, e.g., $\alpha = 3$. If such desired properties fail to hold, there has been no theory on the full or partial regularization of LSQR.

As a windfall, making use of our analysis approach used for CGME, we improve a fundamental bound, Theorem 9.3 presented in Halko et al. [16], for the accuracy of the truncated rank $k$ approximation to $A$ generated by randomized algorithms, which have formed a highly intensive topic over the years. As remarked by Halko et al. in [16] (cf. Remark 9.1 there), their bound appears “conservative, but a complete theoretical understanding lacks.” Our new bounds are sharper than theirs and reveal how the truncation step damages the accuracy of the rank $k$ approximation.

In this paper, we establish a number of regularization properties of CGME and LSMR under the assumption that all the singular values $\sigma_i$ are simple. We prove that the regularization ability of CGME is generally inferior to that of LSQR, that is, the 2-norm filtering best regularized solutions obtained by CGME at semi-convergence are generally less accurate than those obtained by LSQR. We derive the filtered SVD expansion of CGME iterates and prove that the semi-convergence of CGME always occurs no later than that of LSQR and can be much earlier than the latter. Particularly, we show that CGME is not a good choice for $A$ rectangular. We prove that the regularization ability of LSMR is as good as that of LSQR and its semi-convergence occurs no sooner than that of LSQR.

The paper is organized as follows. In Section 2, we review LSQR, CGME, and LSMR. In Section 3, we review some results on LSQR in [32–34]. In Section 4, we derive a number of regularization properties of CGME. In Section 5, we present sharper bounds for the accuracy of the truncated rank $k$ randomized approximation [16]. In Section 6, we study the regularization ability of LSMR. In Section 7, we report numerical experiments to confirm our theory. We conclude the paper in Section 8.

Throughout the paper, we denote by $K_k(C, w) = \text{span}\{w, Cw, \ldots, C^{k-1}w\}$ the $k$ dimensional Krylov subspace generated by the matrix $C$ and the vector $w$, and by the bold letter $0$ the zero matrix with orders clear from the context.

2 The LSQR, CGME, and LSMR algorithms

These three algorithms are all based on the Golub-Kahan bidiagonalization process that computes two orthonormal bases $\{q_1, q_2, \ldots, q_k\}$ and $\{p_1, p_2, \ldots, p_{k+1}\}$ of $K_k(A^T A, A^T b)$ and $K_{k+1}(AA^T, b)$ for $k = 1, 2, \ldots, n$, respectively. We describe the process as Algorithm 1.
Define $P_{k+1} = (p_1, p_2, \ldots, p_{k+1})$, $Q_k = (q_1, q_2, \ldots, q_k)$ and

$$B_k = \begin{pmatrix} 
\alpha_1 & \beta_2 & \alpha_2 \\
\beta_3 & \ddots & \ddots \\
& \ddots & \alpha_k \\
& & \beta_{k+1}
\end{pmatrix} \in \mathbb{R}^{(k+1)\times k}. \quad (2.1)$$

Algorithm 1 can be written in the matrix form

$$AQ_k = P_{k+1}B_k, \quad (2.2)$$

$$A^T P_{k+1} = Q_k B_k^T + \alpha_{k+1} q_{k+1} (e_{k+1})^T, \quad (2.3)$$

where $e_{k+1}$ denotes the $(k + 1)$-th canonical basis vector of $\mathbb{R}^{k+1}$. It is known from (2.2) that

$$B_k = P_{k+1}^T A Q_k. \quad (2.4)$$

The singular values $\theta_i^{(k)}$, $i = 1, 2, \ldots, k$ of $B_k$, called the Ritz values of $A$ with respect to the left and right subspaces span{$P_{k+1}$} and span{$Q_k$}, are all simple.

Write $V_k^R = K_k (A^T A, A^T b)$ and $\beta_1 = \|b\|$. At iteration $k$, LSQR [41] solves

$$\|Ax_{lsqr} - b\| = \min_{x \in V_k^R} \|Ax - b\|$$

for the iterate

$$x_{lsqr} = Q_k y_{lsqr} \quad \text{with} \quad y_{lsqr} = \arg \min_{y \in \mathbb{R}^k} \|B_k y - \beta_1 e_1^{(k+1)}\| = \beta_1 B_k^T e_1^{(k+1)}, \quad (2.5)$$

where $e_1^{(k+1)}$ is the first canonical basis vector of $\mathbb{R}^{k+1}$, and $\|Ax_{lsqr} - b\| = \|B_k y_{lsqr} - \beta_1 e_1^{(k+1)}\|$ decreases monotonically with respect to $k$.

CGME [4, 17, 18, 28, 29] is the CG method implicitly applied to min $\|AA^T y - b\|$ or $AA^T y = b$ and $x = A^T y$, and it solves the problem

$$\|x_{naive} - x_{cgme}^{cgme}\| = \min_{x \in V_k^R} \|x_{naive} - x\|$$

for the iterate $x_{cgme}^{cgme}$. The error norm $\|x_{naive} - x_{cgme}^{cgme}\|$ decreases monotonically with respect to $k$. Let $\bar{B}_k \in \mathbb{R}^{k \times k}$ be the matrix consisting of the first $k$ rows of $B_k$, i.e.,

$$\bar{B}_k = P_k^T A Q_k. \quad (2.6)$$
Then the CGME iterate
\[ x_{cgm}^k = Q_k y_{cgm}^k \quad \text{with} \quad y_{cgm}^k = \beta_1 \bar{B}^{-1} e_1^{(k)} \] (2.7)
and \( \| A x_{cgm}^k - b \| = \beta_{k+1} | (e_1^{(k)})^T y_{cgm}^k | \) with \( e_1^{(k)} \) the kth canonical vector of \( \mathbb{R}^k \).

LSMR \([4, 11]\) is mathematically equivalent to MINRES \([40]\) applied to the normal equation \( A^T A x = A^T b \) of (1.1), and it solves
\[ \| A^T (b - A x_{lsmr}^k) \| = \min_{x \in \mathcal{V}_k^R} \| A^T (b - A x) \| \]
for the iterate \( x_{lsmr}^k \). The residual norm \( \| A^T (b - A x_{lsmr}^k) \| \) of the normal equation decreases monotonically with respect to \( k \), and the iterate
\[ x_{lsmr}^k = Q_k y_{lsmr}^k \quad \text{with} \quad y_{lsmr}^k = \arg \min_{y \in \mathbb{R}^k} \| (B_k^T B_k + \alpha_{k+1} \beta_1 e_1^{(k+1)})^T y - \alpha_1 \beta_1 e_1^{(k+1)} \|. \] (2.8)

3 Some results on LSQR in \([32–34]\)

From \( \beta_1 e_1^{(k+1)} = P_{k+1}^T b \) and (2.5), we have
\[ x_{lsqr}^k = Q_k B_k^T P_{k+1} b, \] (3.1)
which is the minimum 2-norm solution to the problem that perturbs \( A \) in (1.1) to its rank \( k \) approximation \( P_{k+1} B_k Q_k^T \). Recall that \( \| A - A_k \| = \sigma_{k+1} \). LSQR solves a sequence of problems
\[ \min \| x \| \quad \text{subject to} \quad \| P_{k+1} B_k Q_k^T x - b \| = \min \] (3.2)
for \( x_{lsqr}^k \) starting with \( k = 1 \), where \( A \) in (1.1) is replaced by a rank \( k \) approximation \( P_{k+1} B_k Q_k^T \) of it. If \( P_{k+1} B_k Q_k^T \) is a near best rank \( k \) approximation to \( A \) with an approximate accuracy \( \sigma_{k+1} \) and the singular values \( \theta_i^{(k)} \), \( i = 1, 2, \ldots, k \) of \( B_k \) approximate the first \( k \) large \( \sigma_i \) in natural order for \( k = 1, 2, \ldots, k_0 \), then LSQR has the same regularization ability as the TSVD method and thus has the full regularization \([32]\).

Define
\[ y_{lsqr}^k = \| A - P_{k+1} B_k Q_k^T \|, \] (3.3)
which measures the accuracy of the rank \( k \) approximation \( P_{k+1} B_k Q_k^T \) to \( A \) involved in LSQR. Since the best rank \( k \) approximation \( A_k \) satisfies \( \| A - A_k \| = \sigma_{k+1} \), we have
\[ y_{lsqr}^k \geq \sigma_{k+1}. \]

The author in \([33]\) introduces the definition of a near best rank \( k \) approximation to \( A \). The matrix \( P_{k+1} B_k Q_k^T \) is called a near best rank \( k \) approximation to \( A \) if \( y_{lsqr}^k \) is closer to \( \sigma_{k+1} \) than to \( \sigma_k \):
\[ \sigma_{k+1} \leq y_{lsqr}^k < \frac{\sigma_k + \sigma_{k+1}}{2}. \] (3.4)
Such definition is irreplaceable and cannot be relaxed when considering the precise approximation behavior of the singular values $\theta_i^{(k)}$ of $B_k$; see an explanation in [33].

The author [33] has derived accurate estimates for $\gamma_{lsqr}^k$ and approximation properties of $\theta_i^{(k)}$, $i = 1, 2, \ldots, k$ for the three kinds of ill-posed problems. The results have shown that, for severely and moderately ill-posed problems with suitable $\rho > 1$ and $\alpha > 1$ and for $k = 1, 2, \ldots, k_0$, $P_{k+1}B_kQ_k^T$ must be a near best rank $k$ approximation to $A$, and the $k$ Ritz values $\theta_i^{(k)}$ approximate the large singular values $\sigma_i$ of $A$ in natural order. This means that LSQR has the full regularization for these two kinds of problems with suitable $\rho > 1$ and $\alpha > 1$. However, for moderately ill-posed problems with $\alpha$ close to one and mildly ill-posed problems, $P_{k+1}B_kQ_k^T$ is generally not a near best rank $k$ approximation, and the $k$ Ritz values $\theta_i^{(k)}$ do not approximate the large singular values of $A$ in natural order before the semi-convergence of LSQR.

In particular, the author [33, Theorem 5.1] has shown that

$$\gamma_{lsqr}^k = \|G_k\|$$

with

$$G_k = \begin{pmatrix} \alpha_{k+1} \\ \beta_{k+2} & \alpha_{k+2} \\ \beta_{k+3} & \ddots \\ \vdots & \ddots & \alpha_n \\ \beta_{n+1} \end{pmatrix} \in \mathbb{R}^{(n-k+1) \times (n-k)},$$

(3.6)

$$\alpha_{k+1} < \gamma_{lsqr}^k, \quad \beta_{k+2} < \gamma_{lsqr}^k, \quad k = 1, 2, \ldots, n - 1,$$

(3.7)

$$\gamma_{lsqr}^{k+1} < \gamma_{lsqr}^k, \quad k = 1, 2, \ldots, n - 2.$$  

(3.8)

These notation and results will be frequently used later.

4 The regularization properties of CGME

Note that $P_k^Tb = \beta_1e_1^{(k)}$. We obtain

$$x_{k}^{cgme} = Q_k\tilde{B}_k^{-1}P_k^Tb.$$  

(4.1)

Therefore, analogously to (3.2), CGME solves a sequence of problems

$$\min \|x\| \quad \text{subject to} \quad \|P_k\tilde{B}_kQ_k^T x - b\| = \min$$

for the regularized solution $x_{k}^{cgme}$ starting with $k = 1$, where $A$ in (1.1) is replaced by a rank $k$ approximation $P_k\tilde{B}_kQ_k^T$ of it.

Just as LSQR, if $P_k\tilde{B}_kQ_k^T$ is a near best rank $k$ approximation to $A$ and the $k$ singular values of $\tilde{B}_k$ approximate the large ones of $A$ in natural order for $k = 1, 2, \ldots, k_0$, then CGME has the full regularization.
By (2.2), (2.3), and (2.4), the rank $k$ approximation involved in LSQR is

$$P_{k+1}B_k Q_k^T = AQ_k Q_k^T.$$  \(4.3\)

By (3.3), we have $\gamma_k^{lsqr} = \|A(I - Q_k Q_k^T)\|$. For CGME, by (2.3) and (2.6), we obtain

$$P_{k+1}P_k^T A = P_{k+1}(B_k Q_k^T + \alpha_{k+1} e_{k+1}^T q_{k+1}^T)$$

$$= P_{k+1}(B_k, \alpha_{k+1} e_{k+1}^T) Q_k^{T}$$

$$= P_{k+1}B_k Q_k^{T}.$$  \(4.4\)

Therefore, $x_k^{cgme}$ is the solution to (4.2) in which the rank $k$ approximation to $A$ is $P_k B_k Q_k^T = P_k P_k^T A$, whose approximation accuracy is

$$\gamma_k^{cgme} = \|A - P_k B_k Q_k^T\| = \|(I - P_k P_k^T)A\|.$$  \(4.5\)

**Theorem 1** For the rank $k$ approximations $P_k P_k^T A = P_k B_k Q_k^T$ to $A$, $k = 1, 2, \ldots, n - 1$, with the definition $\gamma_0^{lsqr} = \|A\|$, we have

$$\gamma_k^{lsqr} < \gamma_k^{cgme} < \gamma_k^{lsqr}_1,$$  \(4.6\)

$$\gamma_{k+1}^{cgme} < \gamma_k^{cgme}.$$  \(4.7\)

**Proof** It is easily justified from [3, p.304–5] that Algorithm 1 can be run to completion since the singular values of $A$ are all simple and $b$ has nonzero components in all the left singular vectors $u_i$ of $A$. Taking $k = n$ in (2.4) and augmenting $P_{n+1}$ such that $P = (P_{n+1}, \hat{P}) \in \mathbb{R}^{m \times n}$ is orthogonal, we have

$$P^T AQ_n = \begin{pmatrix} B_n \\ 0 \end{pmatrix},$$  \(4.8\)

where all the entries $\alpha_i$ and $\beta_i + 1, i = 1, 2, \ldots, n$, of $B_n$ are positive, and $Q_n \in \mathbb{R}^{n \times n}$ is orthogonal. Then by the orthogonal invariance of the 2-norm, we obtain

$$\gamma_k^{cgme} = \|A - P_k B_k Q_k^T\| = \|P^T (A - P_k B_k Q_k^T) Q_n\| = \|(\beta_{k+1} e_1, G_k)\|$$  \(4.9\)

with $G_k$ defined by (3.6). It is straightforward to justify that the singular values of $G_k \in \mathbb{R}^{(n-k+1) \times (n-k)}$ strictly interlace those of $(\beta_{k+1} e_1, G_k) \in \mathbb{R}^{(n-k+1) \times (n-k+1)}$ by noting that $(\beta_{k+1} e_1, G_k)^T (\beta_{k+1} e_1, G_k)$ is an unreduced symmetric tridiagonal matrix, from which and $\|G_k\| = \gamma_k^{lsqr}$ the lower bound of (4.6) follows.

Based on (4.9), we can prove the upper bound in (4.6). Observe from (3.6) that $(\beta_{k+1} e_1, G_k)$ is the matrix obtained by deleting the first row of $G_{k-1}$. Applying the strict interlacing property of singular values to $(\beta_{k+1} e_1, G_k)$ and $G_{k-1}$, we obtain

$$\gamma_{k-1}^{lsqr} = \|G_{k-1}\| > \|(\beta_{k+1} e_1, G_k)\| = \gamma_k^{cgme},$$

which yields the upper bound of (4.6).

From (4.9), notice that $(\beta_{k+2} e_1, G_{k+1})$ is the matrix obtained by deleting the first row of $(\beta_{k+1} e_1, G_k)$ and the first column, which is zero, of the resulting matrix. Applying the strict interlacing property of singular values to $(\beta_{k+2} e_1, G_{k+1})$ and $(\beta_{k+1} e_1, G_k)$ establishes (4.7).

Relation (4.6) indicates that $P_k P_k^T A = P_k \bar{B}_k Q_k^T$ is definitely a less accurate rank $k$ approximation to $A$ than $AQ_k Q_k^T = P_{k+1} B_k Q_k^T$ in LSQR. Relation (4.7) shows the
strict monotonic decreasing property of $\gamma_{k}^{cgme}$. Since $\gamma_{k}^{lsqr} \geq \sigma_{k+1}$ and $\gamma_{k}^{cgme}$ simply lie between $\gamma_{k}^{lsqr}$ and $\gamma_{k}^{lsqr}$, by combining these facts with the results in Section 3, we know that there is no guarantee that $P_{k}B_{k}Q_{k}^{T}$ is a near best rank $k$ approximation to $A$ even for severely and moderately ill-posed problems.

We next investigate the approximation behavior of the $k$ singular values $\bar{\sigma}_{i,k}$ of $\bar{B}_{k}$, $k = 1, 2, \ldots, n$. Before proceeding, we need to distinguish some subtleties when $A$ is rectangular, i.e., $m > n$, and square, i.e., $m = n$, respectively.

For $m > n$, all the $\alpha_{k}$ and $\beta_{k+1}$ are positive, $k = 1, 2, \ldots, n$, and we generate $P_{n+1}$ and $Q_{n}$ at step $n$ with $\alpha_{n+1} = \beta_{n+2} = 0$. By definition (4.4), we have

$$
\bar{B}_{n+1} = (B_{n}, \alpha_{n+1}e_{n+1}^{(n+1)}) = (B_{n}, 0).
$$

It is known from (4.8) that the singular values of $B_{n}$ are identical to the singular values $\sigma_{i}$, $i = 1, 2, \ldots, n$ of $A$. Therefore, the $n + 1$ singular values of $\bar{B}_{n+1}$ are $\sigma_{i}$, $i = 1, 2, \ldots, n$ and zero.

For $m = n$, however, we must have $\beta_{n+1} = 0$, that is, the last row of $B_{n}$ is zero; otherwise, we would obtain an $n \times (n + 1)$ orthonormal matrix $P_{n+1}$. We have

$$
\bar{B}_{n} = P_{n}^{T}A^{Q_{n}},
$$

whose singular values $\tilde{\sigma}_{i}^{(n)}$, $i = 1, 2, \ldots, n$ are the singular values $\sigma_{i}$ of $B_{n}$, which are identical to the $n$ singular values $\sigma_{i}$ of $A$.

By the definition (4.4) of $\bar{B}_{k}$, from (2.3) and the above description, for both the rectangular and square cases, we obtain

$$
P_{k}^{T}A^{T}P_{k} = \bar{B}_{k}^{T}\bar{B}_{k}, k = 1, 2, \ldots, n^{*},
$$

with $n^{*} = n$ for $m = n$ and $n^{*} = n + 1$ for $m > n$, which are unreduced symmetric tridiagonal matrices. For $m = n$, the eigenvalues of $A^{T}$ are just $\sigma_{i}^{2}$, $i = 1, 2, \ldots, n$, all of which are simple and positive; for $m > n$, the eigenvalues of $A^{T}$ are $\sigma_{i}^{2}$, $i = 1, 2, \ldots, n$ plus $m - n$ zeros, denoted by $\sigma_{n+1}^{2} = \cdots = \sigma_{m}^{2} = 0$ for our later use. Therefore, by the definition of $n^{*}$, the eigenvalues of $\bar{B}_{n^{*}}B_{n^{*}}^{T}$ are $\sigma_{i}^{2}$, $i = 1, 2, \ldots, n^{*}$.

Notice that $\bar{B}_{k}^{T}\bar{B}_{k}$ is nothing but the projection matrix of $A^{T}$ onto the $k$ dimension Krylov subspace $K_{k}(AA^{T}, b)$ and it is generated by the $k$-step symmetric Lanczos tridiagonalization process applied to $A^{T}$ starting with $p_{1} = b/\|b\|$. Therefore, the eigenvalues of $\bar{B}_{k}^{T}\bar{B}_{k}$ approximate some eigenvalues of $A^{T}$ [3, 4, 42].

Particularly, the smallest eigenvalue $(\tilde{\sigma}_{k}^{(k)})^{2}$ of $\bar{B}_{k}^{T}\bar{B}_{k}$ will converge to the smallest one of $A^{T}$ as $k$ increases, which is $\sigma_{n+1}^{2} = 0$ for $m > n$ and $\sigma_{n}^{2} > 0$ for $m = n$. This feature of $\bar{B}_{k}$ is fundamentally different from that of $B_{k}$, whose smallest singular value $\theta_{k}^{(k)} > \sigma_{n}$ unconditionally until $\theta_{n}^{(k)} = \sigma_{n}$ by noticing that $Q_{k}^{T}A^{T}AQQ_{k} = B_{k}^{T}B_{k}$ is the unreduced symmetric tridiagonal matrix generated by the symmetric Lanczos tridiagonalization process applied to $A^{T}A$ starting with $q_{1} = A^{T}b/\|A^{T}b\|$.

We next establish a number of close relationships between $\tilde{\sigma}_{i}^{(k)}$ and $\sigma_{i}$ as well as between them and the singular values $\sigma_{i}$ of $A$. The results play a key role in assessing the regularizing effects of CGME.
Theorem 2 Denote by $\bar{\theta}_i^{(k)}$ and $\theta_i^{(k)}$, $i = 1, 2, \ldots, k$ the singular values of $\bar{B}_k$ and $B_k$, respectively, labeled in decreasing order. Then
\[
\theta_1^{(k)} > \bar{\theta}_1^{(k)} > \theta_2^{(k)} > \bar{\theta}_2^{(k)} > \cdots > \theta_k^{(k)} > \bar{\theta}_k^{(k)}, \quad k = 1, 2, \ldots, n - 1, \tag{4.12}
\]
and
\[
\sigma_n < \bar{\theta}_k^{(k)} < \theta_k^{(k)} < \sigma_k, \quad k = 1, 2, \ldots, n - 1 \tag{4.13}
\]
for $m = n$ and
\[
\sigma_n < \bar{\theta}_k^{(k)} < \theta_k^{(k)} < \sigma_k, \quad k = 1, 2, \ldots, n - 1, \tag{4.14}
\]
\[
0 < \bar{\theta}_k^{(k)} < \theta_k^{(k)} < \sigma_k, \quad k = 1, 2, \ldots, n - 1 \tag{4.15}
\]
for $m > n$.

Proof Note that $\bar{B}_k$ consists of the first $k$ rows of $B_k$ and all the $\alpha_k$ and $\beta_k + 1$ are positive for $k = 1, 2, \ldots, n - 1$. By the strict interlacing property of singular values, we obtain (4.12).

On the other hand, note that, for $A$ both rectangular and square, the singular values of $B_n$ are identical to the ones of $A$, i.e., $\theta_i^{(n)} = \sigma_i$, $i = 1, 2, \ldots, n$. Since $B_k$ consists of the first $k$ columns of $B_n$ and deletes the last $n - k$ zero rows of the resulting matrix, applying the strict interlacing property of singular values to $B_k$ and $B_n$ [43, p. 198, Corollary 4.4], for $k = 1, 2, \ldots, n - 1$, we have
\[
\sigma_{n-k+i} < \bar{\theta}_i^{(k)} < \sigma_i, \quad i = 1, 2, \ldots, k, \tag{4.16}
\]
from which and the definition of $n^*$ it follows that
\[
\sigma_n < \bar{\theta}_k^{(k)} < \sigma_k
\]
for $m = n$ and
\[
0 = \sigma_{n+1} < \bar{\theta}_k^{(k)} < \sigma_k
\]
for $m > n$. The above, together with (4.16) and (4.12), yields (4.13)–(4.15).

From Section 3, relations (4.13) and (4.15) indicate that, unlike the $k$ singular values $\theta_i^{(k)}$ of $B_k$, which have been proved to interlace the first $k + 1$ large ones of $A$ and approximate the first $k$ ones in natural order for the severely or moderately ill-posed problems for suitable $\rho > 1$ or $\alpha > 1$ [33], the lower bound for $\bar{\theta}_k^{(k)}$ is simply $\sigma_n$ for $m = n$ and zero for $m > n$, respectively, and there does not exist a better lower bound for it. This implies that $\bar{\theta}_k^{(k)}$ may be much smaller than $\sigma_{k+1}$ and it can be as small as $\sigma_n$ for $m = n$ and arbitrarily small for $m > n$, independent of $\rho$ or $\alpha$. In other words, the size of $\rho$ or $\alpha$ has no intrinsic effects on the size of $\bar{\theta}_k^{(k)}$, and cannot
make $\tilde{\theta}_i^{(k)}$ lie between $\sigma_{k+1}$ and $\sigma_k$ by choosing $\rho$ or $\alpha$. On the other hand, even if the $\theta_i^{(k)}$ approximate the first $k$ large singular values $\sigma_i$ in natural order, they are less accurate than the $k$ singular values $\theta_i^{(k)}$ of $B_k$ due to (4.13) and (4.15). Consequently, since the $\theta_i^{(k)}$ is always correspondingly larger than the $\tilde{\theta}_i^{(k)}$, the regularization ability of CGME is inferior to that of the LSQR. A final note is that, unlike for $m = n$, CGME may be at risk for $m > n$ since the $\tilde{\theta}_k^{(k)}$ converges to zero other than $\sigma_n$ as $k$ increases and can be arbitrarily small, which causes that the projected problem $\tilde{B}_k y_k^{\text{cgme}} = \beta_1 e_1^{(k)}$ may even be worse conditioned than (1.1) and $\|x_k^{\text{cgme}}\| = \|y_k^{\text{cgme}}\|$ may be unbounded as $k$ increases and bigger than $\|x_{\text{naive}}\|$ for a given (1.1).

In what follows, we establish more results on the regularization of CGME. Recall from, e.g., [22, p. 146] that the LSQR iterate $x_k^{\text{lsgqr}}$ takes the filtered SVD expansion

$$x_k^{\text{lsgqr}} = \sum_{i=1}^{n} f_i^{(k,\text{lsgqr})} \frac{u_i^T b}{\sigma_i} v_i, \quad k = 1, 2, \ldots, n \quad (4.17)$$

with filters

$$f_i^{(k,\text{lsgqr})} = 1 - \prod_{j=1}^{k} \frac{(\theta_j^{(k)})^2 - \sigma_i^2}{(\theta_j^{(k)})^2}, \quad i = 1, 2, \ldots, n. \quad (4.18)$$

These results have been extensively used to study the regularizing effects of LSQR; see, e.g., [22, 23, 32]. We now prove that the CGME solution $x_k^{\text{cgme}}$ also takes a filtered SVD expansion similar to (4.17) and (4.18), but its proof is much more involved.

**Theorem 3** The CGME iterate $x_k^{\text{cgme}}$ has the filtered SVD expansion

$$x_k^{\text{cgme}} = \sum_{i=1}^{n} f_i^{(k,\text{cgme})} \frac{u_i^T b}{\sigma_i} v_i, \quad k = 1, 2, \ldots, n, \quad (4.19)$$

where the filters

$$f_i^{(k,\text{cgme})} = 1 - \prod_{j=1}^{k} \frac{((\tilde{\theta}_j^{(k)})^2 - \sigma_i^2)}{((\tilde{\theta}_j^{(k)})^2)}, \quad i = 1, 2, \ldots, n. \quad (4.20)$$

**Proof** Let $x = A^T y$ and $y_{\text{naive}} = (AA^T)^+ b$ be the naive minimal 2-norm solution to $\min_y \|AA^T y - b\|$. Recall Algorithm 1. For this problem, starting with $y_0^{\text{cgme}} = 0$, at iteration $k$, the CG method extracts $y_k^{\text{cgme}}$ from the $k$ dimensional Krylov subspace

$$\mathcal{K}_k(AA^T, b) = \text{span}\{P_k\}.$$ 

It is well known from, e.g., [38], that the residual of $y_k^{\text{cgme}}$ is

$$b - AA^T y_k^{\text{cgme}} = r_k(AA^T)b, \quad (4.21)$$

where $r_k(\lambda)$ is the $k$th residual, or Ritz, polynomial with the normalization $r_k(0) = 1$, whose $k$ roots are the Ritz values $(\tilde{\theta}_j^{(k)})^2$ of $AA^T$ with respect to $\text{span}\{P_k\}$; see (4.11).
Numerical Algorithms

That is, we have

\[ r_k(\sigma_i^2) = \prod_{j=1}^{k} \frac{(\bar{\theta}_j^{(k)})^2 - \sigma_i^2}{(\bar{\theta}_j^{(k)})^2}, \quad i = 1, 2, \ldots, n. \]  

(4.22)

From the full SVD (1.4) of A, write \( U = (U_n, U_\perp) \). Then we have \( A = U_n \Sigma V^T \), the compact SVD of A. It is straightforward to see that

\[ AA^T(AA^T)^\dagger = (AA^T)^\dagger AA^T = U_n U_n^T. \]

Therefore, by \( y_{\text{naive}} = (AA^T)^\dagger b \), premultiplying the two sides of (4.21) by \((AA^T)^\dagger\) yields

\[ y_{\text{naive}} - U_n U_n^T y_k^{cgme} = (AA^T)^\dagger r_k(AA^T)b \]
\[ = r_k(AA^T)(AA^T)^\dagger b = r_k(AA^T)y_{\text{naive}}, \]

from which it follows that

\[ U_n U_n^T y_k^{cgme} = (I - r_k(AA^T))y_{\text{naive}}. \]  

(4.23)

By the SVD (1.4) of A, we have

\[ y_{\text{naive}} = (AA^T)^\dagger b = \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i^2} u_i. \]

Hence, for \( k = 1, 2, \ldots, n \) from (4.22) and (4.23), we obtain

\[ U_n U_n^T y_k^{cgme} = \sum_{i=1}^{n} (1 - r_k(\sigma_i^2)) \frac{u_i^T b}{\sigma_i^2} u_i \]
\[ = \sum_{i=1}^{n} f_i^{(k,cgme)} \frac{u_i^T b}{\sigma_i^2} u_i \]

(4.24)

with \( f_i^{(k,cgme)} \) defined by (4.20). In terms of \( x_k^{cgme} = A^T y_k^{cgme} \) and \( A = U_n \Sigma V^T \), premultiplying the two sides of the above relation by \( A^T \) and exploiting \( U_n^T U_n = I \), we have

\[ x_k^{cgme} = A^T y_k^{cgme} = V \Sigma U_n^T y_k^{cgme} = V \Sigma U_n^T U_n U_n^T y_k^{cgme} = A^T U_n U_n^T y_k^{cgme}. \]

Then making use of this relation, \( A^T u_i = \sigma_i v_i \) and (4.24), we obtain (4.19).

Based on Theorems 2–3, we can prove the following important result.

**Theorem 4** Let \( k_{cgme}^* \) and \( k_{lsqr}^* \) be iterations at which the semi-convergence of CGME and LSQR occurs, respectively, \( k_0 \) the transition point of the TSVD method. Then

\[ k_{cgme}^* \leq k_{lsqr}^* \leq k_0, \]  

(4.25)

that is, the semi-convergence of CGME occurs no later than LSQR and the TSVD method do.
Proof The result $k^*_{lsqr} \leq k_0$ has been proved in [32, Theorem 3.1]. Next we first prove that $k^*_{cgme} \leq k_0$.

Recall that the best TSVD solution is given by

$$x^*_k = A_k^\dagger b = \sum_{i=1}^{k_0} \frac{u_i^T b}{\sigma_i} v_i$$

and the fact that a 2-norm filtering best possible solution must capture the $k_0$ dominant SVD components of $A$ and suppress the $n - k_0$ small SVD components of $A$.

For CGME, from (4.13) and (4.15), we have $\bar{\theta}_k^{(k)} < \sigma_k$. Therefore, at iteration $k_0 + 1$, we must have $\bar{\theta}_{k_0+1}^{(k_0+1)} < \sigma_{k_0+1}$. If the $\bar{\theta}_i^{(k)}$ approximate the large $\sigma_i$ in natural order for $k = 1, 2, \ldots, k_0$, then by (4.20), we have $f_i^{(k, cgme)} \rightarrow 1$ for $i = 1, 2, \ldots, k$ and $f_i^{(k, cgme)} \rightarrow 0$ for $i = k + 1, \ldots, n$. On the other hand, by (4.20), we have $f_i^{(k_0+1, cgme)} = O(1)$. As a result, $x^*_k$ improves until iteration $k_0$, and the semi-convergence of CGME occurs at iteration $k^*_{cgme} = k_0$.

If the $\bar{\theta}_j^{(k)}$ does not converge to the large singular values of $A$ in natural order and $\bar{\theta}_k^{(k)} < \sigma_{k_0+1}$ for some iteration $k \leq k_0$ for the first time, then $x^*_k$ is already deteriorated by the noise $e$ before iteration $k$: Suppose that $\sigma_{j^*} < \bar{\theta}_k^{(k)} < \sigma_{k_0+1}$ with $j^*$ the smallest integer $j^* > k_0 + 1$. Then we can easily justify from (4.20) that $f_i^{(k, cgme)} \in (0, 1)$ and tends to zero monotonically for $i = j^*, j^* + 1, \ldots, n$, but

$$\prod_{j=1}^{k} \frac{(\bar{\theta}_j^{(k)})^2 - \sigma_i^2}{(\bar{\theta}_j^{(k)})^2} \leq 0, \quad i = k_0 + 1, \ldots, j^* - 1$$

since the first factor is non-positive and the second factor is positive by noting that $\bar{\theta}_j^{(k)} > \sigma_i$, $j = 1, 2, \ldots, k - 1$ for $i = k_0 + 1, \ldots, j^* - 1$. As a result, $f_i^{(k, cgme)} \geq 1$ for $i = k_0 + 1, \ldots, j^* - 1$, showing that $x^*_k$ has been deteriorated by the noise $e$ and the semi-convergence of CGME has occurred at some iteration $k^*_{cgme} < k_0$.

Finally, we prove $k^*_{cgme} \leq k^*_{lsqr}$. Notice that $\bar{\theta}_k^{(k)} < \sigma_k$ means that the first iteration $k$ such that $\bar{\theta}_k^{(k)} < \sigma_{k_0+1}$ for CGME is no more than the one such that $\theta_k^{(k)} < \sigma_{k_0+1}$ for LSQR. Therefore, it is straightforward that the semi-convergence of CGME occurs no later than that of LSQR, i.e., $k^*_{cgme} \leq k^*_{lsqr}$.

It is seen from the above proof that, due to $\bar{\theta}_k^{(k)} < \theta_k^{(k)}$, the semi-convergence of CGME can occur much earlier than that of LSQR.

We can, informally, deduce more features of CGME. By definition, the optimality of CGME means that

$$||x_{naive} - x^*_k|| \leq ||x_{naive} - x^*_{lsqr}|| \tag{4.26}$$

for $i = 1, 2, \ldots, n$ holds unconditionally. Since the noise $e$ does not affect the convergence of CGME and LSQR until their respective semi-convergence, for $k$ no more than the iteration step at which the respective semi-convergence of CGME and LSQR
obtained \( \|x_k - x_{cgme}^k\| \) and \( \|x_k - x_{lsqr}^k\| \) are negligible relative to \( \|x_{naive} - x_{true}\| \), which is supposed very large in the context of discrete ill-posed problems. As a consequence, we have

\[
\|x_{naive} - x_{cgme}^k\| = \|x_{naive} - x_{true} + x_{true} - x_{cgme}^k\|
\approx \|x_{naive} - x_{true}\| + \|x_{true} - x_{cgme}^k\|, \tag{4.27}
\]

\[
\|x_{naive} - x_{lsqr}^k\| = \|x_{naive} - x_{true} + x_{true} - x_{lsqr}^k\|
\approx \|x_{naive} - x_{true}\| + \|x_{true} - x_{lsqr}^k\|. \tag{4.28}
\]

Since the first terms in the right-hand sides of (4.27) and (4.28) are the same constant, by combining (4.26), (4.27), and (4.28), the relation

\[
\|x_{true} - x_{cgme}^k\| \leq \|x_{true} - x_{lsqr}^k\| \tag{4.29}
\]

generally holds until the semi-convergence of CGME. That is, \( x_{k}^{cgme} \) is at least as accurate as \( x_{k}^{lsqr} \) until the semi-convergence of CGME. Afterwards, according to Theorem 4, \( x_{k}^{lsqr} \) continues approximating \( x_{true} \) as \( k \) increases until the occurrence of its semi-convergence, at which LSQR ultimately computes a more accurate approximation to \( x_{true} \). The experiments in [18, 29] have actually confirmed this property. We will demonstrate it by more numerical experiments.

Observe that after Golub-Kahan bidiagonalization is run \( k \) steps, we have already obtained \( \tilde{B}_{k+1}, P_{k+1}, \) and \( Q_{k+1} \). Since \( \alpha_{k+1} > 0 \) for \( k \leq n - 1 \), applying the strict interlacing property of singular values to \( \tilde{B}_k \) and \( \tilde{B}_{k+1} \), we have

\[
\tilde{\theta}_1^{(k+1)} > \tilde{\theta}_2^{(k+1)} > \cdots > \tilde{\theta}_k^{(k+1)} > \tilde{\theta}_{k+1}^{(k+1)}, \quad k = 1, 2, \ldots, n - 1. \tag{4.30}
\]

Note from (4.15) that \( \tilde{\theta}_i^{(k)} < \sigma_i, \quad i = 1, 2, \ldots, k+1 \). Combining (4.30) with (4.15), we see that as approximations to the first large \( k \) singular values \( \sigma_i \) of \( A \), although the \( k \) singular values \( \tilde{\theta}_i^{(k)} \) of \( \tilde{B}_k \) are less accurate than the singular values \( \theta_i^{(k)} \) of \( B_k \), the first \( k \) singular values \( \tilde{\theta}_i^{(k+1)} \) of \( \tilde{B}_{k+1} \) are more accurate than the \( \theta_i^{(k)} \) correspondingly.

Based on the above property and (4.4), we next show how to extract a best possible rank \( k \) approximation to \( A \) from the available rank \( k + 1 \) matrix \( P_{k+1} \tilde{B}_{k+1} Q_{k+1}^T = P_{k+1} P_{k+1}^T A \) generated by Algorithm 1.

**Theorem 5** Let \( \tilde{C}_k \) be the best rank \( k \) approximation to \( \tilde{B}_{k+1} \) with respect to the 2-norm. Then for \( k = 1, 2, \ldots, n - 1 \) we have

\[
\|A - P_{k+1} \tilde{C}_k Q_{k+1}^T\| \leq \tilde{\theta}_{k+1}^{(k+1)} + \gamma_{cgme}^{k+1}, \tag{4.31}
\]

where \( \tilde{\theta}_{k+1}^{(k+1)} \) is the smallest singular value of \( \tilde{B}_{k+1} \) and \( \gamma_{cgme}^{k+1} \) is defined by (4.5).

**Proof** Write \( A - P_{k+1} \tilde{C}_k Q_{k+1}^T = A - P_{k+1} \tilde{B}_{k+1} Q_{k+1}^T + P_{k+1} (\tilde{B}_{k+1} - \tilde{C}_k) Q_{k+1}^T \). Then exploiting (4.4), we obtain

\[
\|A - P_{k+1} \tilde{C}_k Q_{k+1}^T\| \leq \|A - P_{k+1} \tilde{B}_{k+1} Q_{k+1}^T\| + \|P_{k+1} (\tilde{B}_{k+1} - \tilde{C}_k) Q_{k+1}^T\|. \tag{4.32}
\]
Since $P_{k+1}$ and $Q_{k+1}$ are column orthonormal and $C_k$ is the best rank $k$ approximation to $\tilde{B}_{k+1}$, by the orthogonal invariance of 2-norm, we obtain
\[
\|P_{k+1}(\tilde{B}_{k+1} - \tilde{C}_k)Q_{k+1}^T\| = \|\tilde{B}_{k+1} - \tilde{C}_k\| = \tilde{\theta}_{k+1}^{(k+1)},
\]
which, together with (4.32), yields (4.31).

The above proof approach of Theorem 5 will serve the next section.

5 The accuracy of truncated rank $k$ approximate SVDs by randomized algorithms

In this section, we deviate from the context of Krylov solvers and consider the accuracy of a truncated rank $k$ SVD approximation to $A$ constructed by standard randomized algorithms and their improved variants [16]. This topic has been intensively investigated in recent years; see the survey paper [16] and the references therein. Algorithm 2 is one of the two basic randomized algorithms from [16] for computing an approximate SVD and extracting a truncated rank $k$ approximate SVD from it. A minor difference from the other sections in this paper is that we drop the restrictions that the singular values of $A$ are simple and $m \geq n$, that is, the singular values of $A$ are $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{\min\{m,n\}}$.

Algorithm 2 Randomized approximate SVD of $A$.

Input: Given $A \in \mathbb{R}^{m \times n}$, a target rank $k$, and an oversampling parameter $p$ satisfying $\ell = k + p \leq \min\{m, n\}$.

Output: a truncated rank $k$ approximate SVD $A_{(k)}$ of $A$.

Stage A

1. Draw an $n \times \ell$ Gaussian random matrix $\Omega$.
2. Form the $m \times \ell$ matrix $Y = A\Omega$.
3. Compute the compact QR factorization $Y = PR$.

Stage B

1. Form $B = P^T A$.
2. Compute the compact SVD of the $\ell \times n$ matrix $B$: $B = \tilde{U}\tilde{\Sigma}\tilde{V}^T$.
3. Set $\hat{U} = P\tilde{U}$. Compute a rank $\ell$ SVD approximation $PP^TA = \tilde{U}\tilde{\Sigma}\tilde{V}^T$ to $A$.
4. Let $B_{(k)} = \hat{U}_k\hat{\Sigma}_{(k)}\hat{V}_k^T$ be the best rank $k$ approximation to $B$ with the diagonal $\hat{\Sigma}_{(k)}$ being the first $k$ diagonals of $\hat{\Sigma}$, and $\hat{U}_k$ and $\hat{V}_k$ the first $k$ columns of $\hat{U}$ and $\hat{V}$, respectively. Form a truncated rank $k$ SVD approximation $A_{(k)} = PB_{(k)} = \hat{U}_k\hat{\Sigma}_{(k)}\hat{V}_k^T$ to $A$ with $\hat{U}_k = P\hat{U}_k$.

For the approximation accuracy of $A_{(k)}$ to $A$, Halko et al. [16] establish a fundamental result (cf. Theorem 9.3 there):
\[
\|A - A_{(k)}\| \leq \sigma_{k+1} + \|(I - PP^T)A\|. \tag{5.1}
\]
Assume that the oversampling parameter \( p \geq 4 \). Making use of the probability theory, in terms of \( \sigma_{k+1} \), Halko et al. [16] have established a number of bounds for \( \| (I - PP^T)A \| \); see, e.g., Theorems 10.5–10.8 and Corollary 10.9–10.10 there. However, concerning (5.1), they point out in Remark 9.1 that “In the randomized setting, the truncation step appears to be less damaging than the error bound of Theorem 9.3 suggests, but we currently lack a complete theoretical understanding of its behavior.” That is to say, the first term \( \sigma_{k+1} \) in (5.1) is generally conservative and an overestimate.

Motivated by the proof of (4.31), we can improve (5.1) substantially and reveal why (5.1) is an overestimate. Let

\[
\tilde{\sigma}_1 \geq \tilde{\sigma}_2 \geq \cdots \geq \tilde{\sigma}_{k+p} \tag{5.2}
\]

be the singular values of \( B = P^T A \) defined in Algorithm 2. Moreover, we have

\[
P^T AA^T P = BB^T,
\]

which is an \((k + p) \times (k + p)\) symmetric matrix, which is the projection matrix of \( AA^T \) onto the subspace \( \text{span}[P] \) in the orthonormal basis of \( \{p_i\}_{i=1}^{k+p} \) with \( P = (p_1, p_2, \ldots, p_{k+p}) \), whose eigenvalues are \( \tilde{\sigma}_i^2, \ i = 1, 2, \ldots, k + p \). Keep in mind that the eigenvalues of \( AA^T \) are \( \sigma_i^2, \ i = 1, 2, \ldots, \min\{m, n\} \) and \( m - \min\{m, n\} \) zeros, denoted by \( \sigma_{\min\{m,n\}+1}^2 = \cdots = \sigma_m^2 = 0 \) for later use.

**Theorem 6** For \( A \in \mathbb{R}^{m \times n} \), let \( P \) and \( A(k) \) be defined as in Algorithm 2, and \( \tilde{\sigma}_{k+1} \) defined as in (5.2). Then

\[
\| A - A(k) \| \leq \tilde{\sigma}_{k+1} + \| (I - PP^T)A \| \tag{5.3}
\]

with

\[
\sigma_{m-p+1} \leq \tilde{\sigma}_{k+1} \leq \sigma_{k+1}. \tag{5.4}
\]

**Proof** Since \( P \) is orthonormal, the eigenvalues of \( BB^T \) interlace those of \( AA^T \) and satisfy (cf. [43, p.198, Corollary 4.4])

\[
\sigma_{m-(k+p)+i} \leq \tilde{\sigma}_i \leq \sigma_i, \ i = 1, 2, \ldots, k + p,
\]

from which (5.4) follows.

From Algorithm 2, we can write

\[
A - A(k) = A - PP^T A + PP^T A - A(k)
\]

\[
= A - PP^T A + \tilde{U} \tilde{\Sigma} \tilde{V}^T - P \tilde{U}_k \tilde{\Sigma}_k \tilde{V}_k^T
\]

\[
= (I - PP^T)A + P(\tilde{U} \tilde{\Sigma} \tilde{V}^T - \tilde{U}_k \tilde{\Sigma}_k \tilde{V}_k^T).
\]
Since $B(k)$ is the best rank $k$ approximation to $B$, by the column orthonormality of $P$, we obtain

$$
\|A - A(k)\| \leq \|(I - PP^T)A\| + \|P(\tilde{U}\tilde{\Sigma}\tilde{V}^T - \tilde{U}_k\tilde{\Sigma}(k)\tilde{V}^T(k))\|
$$

$$
= \|(I - PP^T)A\| + \|\tilde{U}\tilde{\Sigma}\tilde{V}^T - \tilde{U}_k\tilde{\Sigma}(k)\tilde{V}^T(k)\|
$$

$$
= \|(I - PP^T)A\| + \|B - B(k)\|
$$

$$
= \|(I - PP^T)A\| + \tilde{\sigma}_{k+1}.
$$

**Remark 1** This theorem indicates that $\tilde{\sigma}_{k+1}$ never exceeds $\sigma_{k+1}$ and, for $m, n$ large and $k + p$ small, it may be much smaller than $\sigma_{k+1}$, which can be as small as $\sigma_{m-p+1}$. For $m > n$, whenever $m - p + 1 > n$, we have $\sigma_{m-p+1} = 0$. Thus, bound (5.3) is unconditionally better than bound (5.1) when $\tilde{\sigma}_{k+1} < \sigma_{k+1}$. On the other hand, note that $\sigma_{k+1} \leq \|A - A(k)\|$. Therefore, if $\|(I - PP^T)A\| < \sigma_{k+1}$, we must have $\tilde{\sigma}_{k+1} \approx \sigma_{k+1}$, that is, $\tilde{\sigma}_{k+1}$ dominates bound (5.3). As a result, the truncation step does damage the approximation accuracy of the truncated rank $k$ approximation when $\|(I - PP^T)A\| < \sigma_{k+1}$ and it is less damaging when $\|(I - PP^T)A\| \geq \sigma_{k+1}$.

The column space of $P$ constructed by Algorithm 2 aims to capture the $(k + p)$-dimensional dominant left singular subspace of $A$. The other variant is to capture the $(k + p)$-dimensional right dominant singular subspace of $A$, and it amounts to applying Algorithm 2 to $A^T$ and computes a truncated rank $k$ SVD approximation $A(k)$ to $A$ in a similar way. We call such variant Algorithm 3, and (5.1) becomes

$$
\|A - A(k)\| \leq \sigma_{k+1} + \|A(I - PP^T)\| \quad (5.5)
$$

with the orthonormal $P \in \mathbb{R}^{n \times (k+p)}$.

Note that the eigenvalues of $A^T A$ are $\sigma_i^2$, $i = 1, 2, \ldots, \min\{m, n\}$ and $n - \min\{m, n\}$ zeros, denoted by $\sigma_{\min\{m,n\}+1}^2 = \cdots = \sigma_n^2 = 0$. Since the eigenvalues of $(AP)^T AP$ interlace those of $A^T A$, similarly, we can establish the following result.

**Theorem 7** For $A \in \mathbb{R}^{m \times n}$, let $P$ and $A(k)$ be defined as in Algorithm 3, and $\tilde{\sigma}_1 \geq \tilde{\sigma}_2 \geq \cdots \geq \tilde{\sigma}_{k+p}$ be the singular values of $AP$. Then

$$
\|A - A(k)\| \leq \tilde{\sigma}_{k+1} + \|A(I - PP^T)\| \quad (5.6)
$$

with

$$
\sigma_{n-p+1} \leq \tilde{\sigma}_{k+1} \leq \sigma_{k+1}. \quad (5.7)
$$

**Remark 2** In the case $m < n$, whenever $n - p + 1 > m$, we have $\sigma_{n-p+1} = 0$. Bound (5.6) is unconditionally better and can be substantially sharper than the bound (5.5) for $m, n$ large, and $k + p$ small.

**Remark 3** If the singular values $\sigma_i$ of $A$ are all simple, by the strict interlacing properties of eigenvalues, the singular values of $B$ in Algorithms 2–3 are all simple too, and the lower and upper bounds in (5.4) and (5.7) are strict, i.e., $\tilde{\sigma}_{k+1} < \sigma_{k+1}$.
Remark 4 Relations (5.1) and (5.5) and Theorems 6–7 hold for all the truncated rank 
$k$ SVD approximations generated by the enhanced variants of Algorithm 2–3 in [16],
where the only difference between the variants is the way that $P$ is generated. More
generally, Theorems 6–7 are true for arbitrarily given orthonormal $P \in \mathbb{R}^{m \times (k+p)}$
and $P \in \mathbb{R}^{n \times (k+p)}$ with $k + p \leq \min\{m, n\}$, respectively.

6 The regularization properties of LSRM

From Algorithm 1, we obtain

$$Q_{k+1}^T A^T A Q_k = \left( B_k^T B_k, \alpha_{k+1} \beta_{k+1} e^{(k)}_k \right)^T.$$  \hspace{1cm} (6.1)

Therefore, from (2.8), noting that $Q_{k+1}^T A^T b = \alpha_1 \beta_1 e^{(k+1)}_1$, we have

$$x_{k}^{\text{lsmr}} = Q_k (Q_{k+1}^T A Q_k)^\dagger Q_{k+1}^T A^T b,$$ \hspace{1cm} (6.2)

which means that LSRM solves the problem

$$\min \| x \| \text{ subject to } \| Q_{k+1}^T A^T A Q_k Q_k^T x - A^T b \| = \min$$ \hspace{1cm} (6.3)

for the regularized solution $x_{k}^{\text{lsmr}}$ starting with $k = 1$. In the meantime, it is
straightforward to justify that the TSVD solution $x_{k}^{\text{svd}}$ solves the problem

$$\min \| x \| \text{ subject to } \| A_k^T A x - A^T b \| = \min.$$ \hspace{1cm} (6.4)

In view of (6.3) and (6.4), we need to accurately estimate the approximation accuracy
$\| A^T A - Q_{k+1}^T A^T A Q_k Q_k^T \|$ and investigate how the singular values of
$Q_{k+1}^T A^T A Q_k$ approximate the $k$ large singular values $\sigma_i^2$, $i = 1, 2, \ldots, k$ of $A^T A$.
We are concerned with some intrinsic relationships between the regularizing effects of
LSMR and those of LSQR and compare the regularization ability of the two
methods.

By (3.1), (2.2), (2.3), (2.4), and $P_{k+1} P_{k+1}^T = b$, the LSQR iterate

$$x_k^{\text{lsrc}} = Q_k B_k^\dagger P_{k+1}^T = Q_k (Q_{k+1}^T A Q_k)^-1 Q_k^T P_{k+1}^T$$

which is the solution to the problem

$$\min \| x \| \text{ subject to } \| Q_k Q_k^T A^T A Q_k Q_k^T x - A^T b \| = \min$$ \hspace{1cm} (6.5)

that replaces $A^T A$ by its rank $k$ approximation $Q_k Q_k^T A^T A Q_k Q_k^T = Q_k B_k^T B_k Q_k^T$
in the normal equation $A^T A x = A^T b$. In this sense, the accuracy of such rank $k$
approximation is measured in terms of $\| A^T A - Q_k Q_k^T A^T A Q_k Q_k^T \|$ for LSQR.

Firstly, we present the following result, which compares the accuracy of two rank $k$
approximations involved in LSMR and LSQR in the sense of solving the normal
equation $A^T A x = A^T b$. 

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Theorem 8 For the rank $k$ approximations to $A^T A$ in (6.3) and (6.5) and $k = 1, 2, \ldots, n - 1$, we have

$$
\| A^T A - Q_{k+1}^T A^T A Q_k Q_k^T \| < \| A^T A - Q_k Q_k^T A^T A Q_k Q_k^T \|. 
$$

(6.6)

Proof For the orthogonal matrix $Q_n$ generated by Algorithm 1, noticing that $\alpha_{n+1} = 0$, from (2.2) and (2.3), we obtain

$$
Q_n^T A^T A Q_n = B_n^T B_n
$$

and

$$
\| A^T A - Q_k Q_k^T A^T A Q_k Q_k^T \| = \| Q_n^T (A^T A - Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T) Q_n \|
$$

$$
= \| B_n^T B_n - (I, 0)^T (B_k^T B_k, \alpha_{k+1} \beta_{k+1} e_k)^T (I, 0) \|
$$

$$
= \| F_k \|, \; k = 1, 2, \ldots, n - 1, 
$$

(6.7)

where

$$
F_k = \begin{pmatrix}
\alpha_{k+1} + \beta_{k+1} & \alpha_k + \beta_k \\
\alpha_k + \beta_k & \alpha_{k-1} + \beta_{k-1} & & \\
& \alpha_{k-2} + \beta_{k-2} & & \\
& & \ddots & \\
& & & \alpha_1 + \beta_1 \\
\end{pmatrix}
$$

$$
= \left( \begin{array}{c}
\alpha_{k+1} \beta_{k+1} e_2^{(n-k+1)} \\
G_k^T G_k
\end{array} \right) \in \mathbb{R}^{(n-k+1) \times (n-k)} 
$$

(6.8)

is the matrix obtained by deleting the $(k + 1) \times k$ leading principal matrix of the symmetric tridiagonal matrix $B_n^T B_n$ and the first $k - 1$ zero rows and $k$ zero columns of the resulting matrix, where $G_k$ is defined by (3.6) and $e_1^{(n-k)}$ is the first canonical vector of $\mathbb{R}^{n-k}$.

On the other hand, it is straightforward to verify that

$$
\| A^T A - Q_k Q_k^T A^T A Q_k Q_k^T \| = \| Q_n^T (A^T A - Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T) Q_n \|
$$

$$
= \| B_n^T B_n - (I, 0)^T (B_k^T B_k, \alpha_{k+1} \beta_{k+1} e_k)^T (I, 0) \|
$$

$$
= \| F'_k \|, 
$$

(6.9)

where $F'_k = \begin{pmatrix} \alpha_{k+1} \beta_{k+1} e_2^{(n-k+1)} \end{pmatrix} \in \mathbb{R}^{(n-k+1) \times (n-k)}$ with $e_2^{(n-k+1)}$ being the second canonical vector of $\mathbb{R}^{n-k+1}$.

Since $G_k^T G_k$ is unreduced symmetric tridiagonal, its eigenvalues are all simple. Therefore, from (6.8) and (6.8), we obtain

$$
F'_k (F'_k)^T = (\alpha_{k+1} \beta_{k+1} e_2^{(n-k+1)}, F_k) (\alpha_{k+1} \beta_{k+1} e_2^{(n-k+1)}, F_k)^T
$$

$$
= F_k F_k^T + \alpha_{k+1}^2 \beta_{k+1}^2 e_2^{(n-k+1)} (e_2^{(n-k+1)})^T. 
$$

(6.10)

Since $G_k^T G_k$ is unreduced symmetric tridiagonal, its eigenvalues are all simple. Keep in mind from (3.5) that $\| G_k \| = \gamma_k^{\text{sym}}$, and observe from (6.8) that

$$
F_k^T F_k = (G_k^T G_k)^2 + \alpha_{k+1}^2 \beta_{k+1}^2 e_1^{(n-k)} (e_1^{(n-k)})^T, \; k = 1, 2, \ldots, n - 1. 
$$

(6.11)
Therefore, we know from [7, p. 218] that the eigenvalues of $F_k^T F_k$ strictly interlace those of $(G_k^T G_k)^2$ and are all simple. Furthermore, we see from (3.6) that $G_k$ is of full column rank, which means that the eigenvalues of $F_k^T F_k$ are all positive.

Note that the eigenvalues of $F_k F_k^T$ are those of $F_k^T F_k$ plus a zero. As a result, the eigenvalues of $F_k F_k^T$ are all simple. According to [7, p. 218], we know from (6.10) that the eigenvalues of $F_k'(F_k')^T$ strictly interlace those of $F_k F_k^T$. Therefore, we obtain

$$
\|F_k\|^2 = \|F_k'(F_k')^T\| > \|F_k F_k^T\| = \|F_k\|^2,
$$

which, from (6.7) and (6.9), establishes (6.6).

This theorem indicates that, as far as solving $A^T Ax = A^T b$ is concerned, the rank $k$ approximation in LSMR is more accurate than that in LSQR.

Secondly, recall that (3.3) measures the quality of the rank $k$ approximation involved in LSQR for the regularization problem (3.2). We estimate the approximation accuracy of $Q_k + Q_k^T A Q_k Q_k^T$ to $A^T A$ in terms of $(\gamma^{lsqr}_k)^2$ and prove its monotonic decreasing property.

**Theorem 9** For $k = 1, 2, 3, \ldots, n - 1$, let $\gamma^{lsqr}_k$ be defined as (3.3). For $k = 2, 3, \ldots, n - 1$ we have

$$(\gamma^{lsqr}_k)^2 < \|A^T A - Q_{k+1} Q_{k+1}^T A Q_{k+1} Q_{k+1}^T\| \leq \sqrt{1 + m_k (\gamma^{lsqr}_{k-1}/\gamma^{lsqr}_k)^2 (\gamma^{lsqr}_k)^2}$$

with $0 < m_k < 1$ and $\gamma^{lsqr}_0 = \|A\|$.

For $k = 1, 2, 3, \ldots, n - 2$, the strict monotonic decreasing property holds:

$$\|A^T A - Q_{k+1} Q_{k+1}^T A Q_{k+1} Q_{k+1}^T\| < \|A^T A - Q_{k+2} Q_{k+2}^T A Q_{k+1} Q_{k+1}^T\|.$$  

(6.13)

**Proof** Combining (6.8) with (3.5) and (3.7), for $k = 2, 3, \ldots, n - 1$, we obtain from [46, p. 98] and [7, p. 218] that

$$
\|F_k\|^2 = \|G_k\|^4 + m'_k \alpha^2_{k+1} \beta^2_{k+1} \leq (\gamma^{lsqr}_k)^4 + m_k (\gamma^{lsqr}_{k-1} \gamma^{lsqr}_k)^2
$$

with $0 < m'_k \leq 1$ and $\gamma^{lsqr}_0 = \|A\|$. From (3.7), we have $\alpha_2 < \gamma^{lsqr}_1$, $\beta_2 < \|A\| = \gamma^{lsqr}_0$. Therefore, we obtain

$$(\gamma^{lsqr}_1)^4 < \|F_1\|^2 = \|G_1\|^4 + m'_1 \alpha^2_2 \beta^2_2 \leq (\gamma^{lsqr}_1)^4 + m_1 (\gamma^{lsqr}_0 \gamma^{lsqr}_1)^2,$$

from which it follows that (6.12) holds.

From (6.8), we see that $F_{k+1}$ is the matrix that first deletes the first column and row of $F_k$ and then deletes the first zero column and row of the resulting matrix. Therefore, applying the interlacing property of singular values to $F_{k+1}$ and $F_k$ yields

$$
\|F_k\| \leq \|F_{k+1}\|.
$$

We next prove that the above “$\leq$” is the strict “$<$.” Note that $B_n^T B_n = Q_n^T A^T A Q_n$ is an unreduced symmetric tridiagonal matrix. Therefore, its singular values $\sigma_i^2$, $i = 1, 2, \ldots, n$ are simple. Observe that $F_k$ is the matrix deleting the first $k$ columns of
\[ B_n^T B_n \text{ and the first } k \text{ zero rows of the resulting matrix. Consequently, the singular values } \xi_i^{(k)}, \quad i = 1, 2, \ldots, n - k \text{ of } F_k \text{ strictly interlace the simple singular values } \sigma_i^2, \quad i = 1, 2, \ldots, n \text{ of } B_n^T B_n \text{ and thus must be simple for } k = 1, 2, \ldots, n - 1. \text{ Moreover, the singular values of } F_{k+1} \text{ strictly interlace those of } F_k, \text{ which means that } \xi_1^{(k)} < \xi_1^{(k+1)}, \text{ i.e., } \|F_k\| < \|F_{k+1}\|, \text{ which proves (6.13)}. \]

**Remark 5** According to the results and analysis in [33], we have \( \gamma_{lsqr}^{k-1}/\gamma_{lsqr}^k \sim \rho \) for severely ill-posed problems, and \( \gamma_{lsqr}^k/\gamma_{lsqr}^{k-1} \sim (k/(k - 1))^\alpha \) for moderately and mildly ill-posed problems. Therefore, (6.12) indicates that \( \|A^T A - Q_k^T Q_k + A Q_k^T Q_k\| \sim (\gamma_{lsqr}^k)^2 \).

Finally, let us investigate the relationship between the singular values of rank \( k \) approximation matrices in LSMR and LSQR. From (6.1) and (2.4), we know that they are the singular values of \((B_k^T B_k, \alpha_k + 1 \beta_k + 1 e_k^{(k)})^T\) and \(B_k^T B_k\), respectively.

**Theorem 10** Let \( \tilde{\theta}_4^{(k)} > (\tilde{\theta}_2^{(k)})^2 \cdots > (\tilde{\theta}_1^{(k)})^2 \) be the singular values of \((B_k^T B_k, \alpha_k + 1 \beta_k + 1 e_k^{(k)})^T\). Then for \( i = 1, 2, \ldots, k \) we have
\[
\tilde{\theta}_i^{(k)} < \tilde{\theta}_i^{(k)} < \sigma_i, \quad (6.14)
\]
\[
(\tilde{\theta}_i^{(k)})^2 < (\sigma_i^{(k)})^2 + \gamma_{lsqr}^k \gamma_{lsqr}^{k-1}. \quad (6.15)
\]

**Proof** Observe that \((B_k^T B_k, \alpha_k + 1 \beta_k + 1 e_k^{(k)})^T\) is the matrix consisting of the first \( k \) columns of \( B_n^T B_n \) and deleting the last \( n - k - 1 \) zero rows of the resulting matrix. As a result, since \( \sigma_i, \quad i = 1, 2, \ldots, n \), are simple, the singular values \( (\tilde{\theta}_i^{(k)})^2 \) of \((B_k^T B_k, \alpha_k + 1 \beta_k + 1 e_k^{(k)})^T\) strictly interlace the singular values \( \sigma_i^2 \) of \( B_n^T B_n \):
\[
\sigma_{n-k+i}^2 < (\tilde{\theta}_i^{(k)})^2 < \sigma_i^2, \quad i = 1, 2, \ldots, k,
\]
which means the upper bound (6.14).

Note that \((B_k^T B_k, \alpha_k + 1 \beta_k + 1 e_k^{(k)})^T(B_k^T B_k, \alpha_k + 1 \beta_k + 1 e_k^{(k)})\) has the \( k + 1 \) eigenvalues \((\tilde{\theta}_i^{(k)})^4\) and zero, and \((B_k^T B_k)^T(B_k^T B_k) = (B_k^T B_k)^2\) is its \( k \times k \) leading principal submatrix and has \( k \) simple eigenvalues \((\theta_i^{(k)})^4\). Therefore, \((\theta_i^{(k)})^4\) strictly interlace \((\tilde{\theta}_i^{(k)})^4\) and zero, which proves the lower bound of (6.14).

On the other hand, we have
\[
(B_k^T B_k, \alpha_k + 1 \beta_k + 1 e_k^{(k)})(B_k^T B_k, \alpha_k + 1 \beta_k + 1 e_k^{(k)})^T = (B_k^T B_k)^2 + \alpha_k^2 \beta_k^2 (e_k^{(k)})^T (e_k^{(k)})^T.
\]
Recall (3.6) that \( \alpha_{k+1} < \gamma_{lsqr}^k \) and \( \beta_{k+1} < \gamma_{lsqr}^{k-1} \). By standard perturbation theory, we obtain
\[
(\tilde{\theta}_i^{(k)})^4 - (\theta_i^{(k)})^4 \leq \alpha_k^2 \beta_k^2 (e_k^{(k)})^T (e_k^{(k)})^T, \quad i = 1, 2, \ldots, k,
\]
from which it follows that (6.15) holds.
Remark 6 Equation (6.14) indicates that $\tilde{\theta}_i^{(k)}$, $1 = 1, 2, \ldots, k$ approximate the first $k$ large singular values $\sigma_i$ more accurately than $\theta_i^{(k)}$. Particularly, since $\theta_k^{(k)} < \tilde{\theta}_k^{(k)}$, the first iteration step $k^*$ such that $\tilde{\theta}_k^{(k^*)} < \sigma_{k_0+1}$ must be no smaller than the $k^*$ such that $\theta_k^{(k^*)} < \sigma_{k_0+1}$. This, together with the previous analysis on the semi-convergence of LSQR, implies that the semi-convergence of LSMR must occur no sooner than that of LSQR. On the other hand, (6.15) shows that $\tilde{\theta}_i^{(k)}$ is bounded from above by $\theta_i^{(k)}$ as an approximation to $\sigma_i$, which, together with (6.14), implies that $\tilde{\theta}_i^{(k)}$ and $\theta_i^{(k)}$ interact and one cannot expect that $\theta_i^{(k)}$ is considerably more accurate than $\tilde{\theta}_i^{(k)}$ as approximations to the large singular values of $A$ for $i = 1, 2, \ldots, k$.

Remark 7 Theorem 8 and the above two remarks mean that the regularizing effects of LSMR are not inferior to those of LSQR and the best regularized solutions by LSMR are at least as accurate as those by LSQR, that is, LSMR has the same regularization ability as that of LSQR. Particularly, from the theory of LSQR in Section 3, we conclude that LSMR has the full regularization for severely or moderately ill-posed problems with suitable $\rho > 1$ or $\alpha > 1$.

7 Numerical experiments

All the computations are carried out in Matlab R2017b on the Intel Core i7-4790k with CPU 4.00 GHz processor and 16 GB RAM with the machine precision $\epsilon_{\text{mach}} = 2.22 \times 10^{-16}$ under the Microsoft Windows 8 64-bit system.

We have tested LSQR, CGME, and LSMR on almost all the 1D and 2D problems from [2, 12, 23, 25, 26] and have observed similar phenomena. For the sake of length, we list only some of them in Table 1, where each problem takes its default parameter(s). The 1D problems shaw, gravity and baart are severely ill-posed, phillips and heat are moderately ill-posed, all of which are with the order $5000 \times 5000$, and deriv2 is moderately ill-posed with the order $m = n = 10000$. The 2D problems blur, fanbeamtomo and seismitomo are from [23, 25]. For these three problems, although the orders $m$ and $n$ are already tens of thousands, by using the Matlab built-in function svd to compute singular values only, we find that the ratios $\sigma_1/\sigma_n$ are only 31.5, 2472, and 408.8, respectively, which, intuitively, do not satisfy the definition of a discrete ill-posed problem whose condition number $\sigma_1/\sigma_n$ is large. The other 2D problems are from [2]; for each of which we compute $b_{\text{true}} = Ax_{\text{true}}$ and add a Gaussian white noise $e$ with zero mean to it by prescribing the relative noise level

$$\varepsilon = \frac{\|e\|}{\|b_{\text{true}}\|}. \quad (7.1)$$

We use the code lsqr_b.m of [23], where the reorthogonalization is exploited during Golub-Kahan bidiagonalization in order to maintain the numerical orthogonality of $P_{k+1}$ and $Q_k$. We have written the Matlab codes of CGME and LSMR based on the same Golub-Kahan bidiagonalization process used in lsqr_b.m.

For all the four 1D problems and seismitomo, we report the results for $\varepsilon = 10^{-3}$; for all the other 2D problems except blur and fanbeamtomo, we report the results for...
Table 1 The description of test problems

| Problem           | Description                                | Size of $m, n$ |
|-------------------|--------------------------------------------|----------------|
| shaw              | 1D image restoration model                 | $m = n = 5000$ |
| phillips          | phillips’ famous test problem              | $m = n = 5000$ |
| heat              | Inverse heat problem                       | $m = n = 5000$ |
| deriv2            | Computation of second derivative           | $m = n = 10000$ |
| AtmosphericBlur10 | Spatially Invariant Gaussian Blur          | $m = n = 65536$ |
| AtmosphericBlur30 | Spatially Invariant Gaussian Blur          | $m = n = 65536$ |
| GaussianBlur420   | Spatially Invariant Atmospheric Blur       | $m = n = 65536$ |
| GaussianBlur422   | Spatially Invariant Atmospheric Blur       | $m = n = 65536$ |
| VariantMotionBlur_large | Spatially Variant Motion Blur            | $m = n = 65536$ |
| VariantMotionBlur_medium | Spatially Variant Motion Blur         | $m = n = 65536$ |
| seismictomo       | 2D seismic tomography                      | 20000 $\times$ 10000 |
| blur              | 2D image restoration                       | $m = n = 22500$ |
| fanbeamtomo       | 2D fan-beam tomography problem             | 61200 $\times$ 14400 |

$\epsilon = 5 \times 10^{-3}$. For several other $\epsilon \in [10^{-3}, 5 \times 10^{-2}]$, we have observed similar phenomena for all the problems except blur and fanbeamtomo. For blur and fanbeamtomo, we will report some remarkable distinctions on the convergence features for $\epsilon$ lying in this practical interval. Table 2 displays the results on all the problems but blur, where $\epsilon = 0.05$ for fanbeamtomo. Figures 1, 2, 3, 4, 5, 6, and 7 depict the convergence processes of LSQR, CGME, and LSMR, where the “error” is the relative error of the best regularized solution obtained by each algorithm, which is defined by

$$
\epsilon_{\text{solver}} = \frac{\|x_{k^*}^{\text{solver}} - x_{\text{true}}\|}{\|x_{\text{true}}\|},
$$

Table 2 The results on some problems

| Problem                     | CGME | LSMR | LSQR |
|-----------------------------|------|------|------|
|                             | $k^*$ | $\epsilon_{\text{cgme}}$ | $k^*$ | $\epsilon_{\text{lsmr}}$ | $k^*$ | $\epsilon_{\text{lqsr}}$ |
| shaw                        | 6    | 0.0854 | 9    | 0.0359 | 9    | 0.0359 |
| phillips                    | 4    | 0.0243 | 11   | 0.0046 | 11   | 0.0049 |
| heat                        | 14   | 0.0670 | 24   | 0.0157 | 24   | 0.0160 |
| deriv2                      | 8    | 0.2135 | 23   | 0.1135 | 22   | 0.1146 |
| AtmosphericBlur10           | 27   | 0.1548 | 68   | 0.1337 | 54   | 0.1377 |
| AtmosphericBlur30           | 3    | 0.3179 | 19   | 0.2764 | 15   | 0.2772 |
| VariantMotionBlur_large     | 68   | 0.2813 | 120  | 0.2557 | 106  | 0.2571 |
| VariantMotionBlur_medium    | 68   | 0.2817 | 118  | 0.2567 | 104  | 0.2580 |
| seismictomo                 | 31   | 0.0771 | 160  | 0.0624 | 120  | 0.0633 |
| fanbeamtomo                 | 7    | 0.2995 | 15   | 0.1759 | 13   | 0.1781 |
Fig. 1 a–d 1D problems with the relative noise level $\varepsilon = 10^{-3}$

Fig. 2 a, b AtmosphericBlurxx
where the “solver” is “lsqr,” “cgme,” and “lsmr,” respectively.

We now comment Table 2 and the figures in order.

Firstly, the semi-convergence of CGME occurs earlier than LSQR and can be much earlier. This confirms Theorem 4. The much earlier semi-convergence of CGME indicates that we must have $\bar{\theta}(k^*) < \theta(k^*)$ considerably and LSQR continues improving iterates until the occurrence of its semi-convergence.

Secondly, the best regularized solutions $x_{k^*}^{cgme}$ are correspondingly less accurate than $x_{k^*}^{lsqr}$ considerably except blur in Fig. 4, where the best regularized solution by CGME is almost as accurate as those by LSQR and LSRM. For all the 1D problems and the 2D problem fanbeamtomo with $\varepsilon = 10^{-3}$, the relative errors of the best regularized solutions by CGME are twice to five times larger than the counterparts by LSRM and LSQR, indicating that the regularization ability of CGME is considerably inferior to those of LSRM and LSQR, given that the the relative errors by LSQR and LSRM themselves are only roughly $0.01 \sim 0.1$; see Figs. 7a and 5a. These results confirm Theorems 1–2.
Thirdly, for each of the problems, by a careful observation and comparison, we have found that $x_{k}^{cgme}$ is more accurate and at least not less accurate than $x_{k}^{lsqr}$ until the occurrence of CGME, after which LSQR continues improving iterates until the occurrence of its semi-convergence, as is clearly seen from most of Figs. 1, 2, 3, 4, and 5. For the 1D test problems, by our manual record that is not listed here, we have found that it is also the case though not so obvious from Fig. 7. These results justify our arguments on (4.29).

Fourthly, for each of the 2D problems, the best regularized solution $x_{k}^{lsmr}$ is at least as accurate as $x_{k}^{lsqr}$, and the semi-convergence of LSMR always occurs no sooner and actually later than that of LSQR. We notice that the relative error of $x_{k}^{lsmr}$ is very slightly smaller than that of $x_{k}^{lsqr}$, and there are very little differences between the corresponding counterparts. For all the 1D problems, the semi-convergence of LSMR and LSQR occurs exactly at the same iterations, and the best regularized solutions obtained by them have the same accuracy. These results confirm Remark 6 and justify that LSMR has the same regularization ability as that of LSQR.

Fig. 5  a, b seismictomo with $\epsilon = 10^{-3}$

(a) (b) Blur with $\epsilon = 5 \times 10^{-3}$
Fifthly, for blur and fanbeam tomo with $\varepsilon = 10^{-3}$, Figs. 4 and 5 indicate that there is no semi-convergence phenomenon for LSQR and LSMR, and the TSVD method finds its best regularized solution at $k_0 = n$. This means that $e$ does not play a part in regularization and these methods solve these two problems as if they were a standard linear system and a least squares problem. Furthermore, it is clear from the figures that the relative errors of regularized solutions obtained by LSQR and LSMR stabilize after 30 iterations for blur and 80 iterations for fanbeam tomo, respectively.

Figures 4 and 5 seem to indicate that CGME has semi-convergence phenomena for the rectangular fanbeam tomo and given $\varepsilon$ but it does not have for the square blur. However, this semi-convergence is in disguise and is not caused by the noise $e$: Notice that the matrix $A$ of fanbeam tomo is rectangular, and recall (4.15) in Theorem 2 and its proof as well as the comment paragraph after Theorem 2. We know that the smallest singular value $\tilde{\theta}(k)$ of $\tilde{B}_k$ can be arbitrarily small and approaches zero as $k$ increases as $(\tilde{\theta}(k))^2$ approaches the eigenvalue zero of $AA^T$ as $k$ increases. As a result, the projected problem $\tilde{B}_k y_{k}^{cgme} = \beta e_1^{(k)}$ in CGME can become even worse conditioned than (1.1) itself as $k$ increases for $A$ rectangular, causing that $\|x_k^{cgme}\| = \|Q_k y_k^{cgme}\| = \|y_k^{cgme}\|$ and the relative error $\frac{\|x_k^{cgme} - x_{true}\|}{\|x_{true}\|}$ increase quickly and unboundedly with respect to $k$. This can be seen from (4.20), where we can easily check that $|f_k^{(k, cgme)}| \rightarrow \infty$ as $k$ increases since $\tilde{\theta}(k) \rightarrow 0$ as $k$ increases.

In contrast, the smallest singular values of the projection matrices are always bounded from below by either $\sigma_n$ for LSQR (cf. (4.14)) or $\sigma_n^2$ for LSMR (cf. (6.14)), no matter how $A$ is rectangular or square. This is why CGME has seemingly semi-convergence phenomenon for $A$ rectangular, while LSMR and LSQR do not have. In the meantime, we see that the best regularized solution by CGME is substantially less accurate than those by LSMR and LSQR for fanbeam tomo. For the square blur with $\varepsilon = 10^{-3}$, we see that CGME, LSMR, and LSQR do not exhibit semi-convergence and they compute very comparable approximate solutions with all the
errors $\epsilon_{\text{solver}} \approx 0.4$. These results and analysis tell us that CGME is definitely not a good choice when $A$ is rectangular.

Sixthly, if the relative noise level $\epsilon$ is increased to $\epsilon = 0.05$, the semi-convergence of LSQR and LSMR occurs for fanbeamtomo, but CGME computes a less accurate best regularized solution that LSMR and LSQR do, as Fig. 5b and Table 2 indicate. We have also observed the semi-convergence of the three algorithms and the TSVD method for blur with $\epsilon = 0.05$. We find that the best regularized solutions by LSQR and LSMR have very comparable accuracy but CGME computes a less accurate best regularized solution. We omit the corresponding figure.

8 Conclusions

For a general large-scale ill-posed problem (1.1), the Krylov solvers LSQR, CGLS, CGME, and LSMR have been commonly used. They have general regularizing effects and exhibit semi-convergence. In terms of the accuracy of the rank $k$ approximation to $A$ in LSQR, we have derived accurate estimates for the accuracy of the rank $k$ approximations to $A$ and $A^TA$ that are involved in CGME and LSMR, respectively. We have analyzed the approximation behavior of the singular values of the projection matrices associated with CGME and LSMR, and established a number of results on them. We have also derived the filtered SVD expansion of CGME regularized solutions. Based on them, we have shown that the regularization ability of CGME is generally inferior to that of LSQR and the semi-convergence of CGME occurs no later than that of LSQR. Particularly, we have shown that CGME is not a good method for $A$ rectangular.

In the meantime, we have proved that LSMR has the same regularizing effects as LSQR and the semi-convergence of LSMR occurs no sooner than that of LSQR. Particularly, we have shown that LSMR has the full regularization for severely and moderately ill-posed problems with suitable $\rho > 1$ and $\alpha > 1$. We have made detailed numerical experiments to show the regularization properties of CGME and LSMR.

We have improved a fundamental result, Theorem 9.3 in [16], which gives a bound for the approximation accuracy of the truncated rank $k$ SVD approximation to $A$ generated by randomized algorithms and lacks a complete understanding to its considerable overestimate. Our new bounds are sharper than theirs and reveal how the truncation step affects the accuracy of the truncated rank $k$ approximation to $A$.

We have considered the regularizing effects of CGME and LSQR by assuming that all the singular values of $A$ are simple. Using the regularization results on LSQR and analysis approach in [32, 33], all the results in this paper can be extended to the multiple singular value case for CGME and LSMR, as done in [34] for LSQR.

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