

REGULARIZATION PROPERTIES OF THE 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, there are four commonly used Krylov solvers: LSQR and its mathematically equivalent CGLS, the Conjugate Gradient (CG) method applied to $A^T Ax = A^T b$, CGME, the CG method applied to $\min \|AA^T y - b\|$ or $AA^T y = b$ with $x = A^T y$, and LSMR, 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 establish a number of regularization properties of CGME and LSMR, including the filtered SVD expansion of CGME iterates, and prove that the 2-norm filtering best 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.

Key words. Discrete ill-posed, rank k approximations, semi-convergence, regularized solution, Lanczos bidiagonalization, TSVD regularized solution, CGME, LSMR, LSQR, CGLS

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1. Introduction and Preliminaries. Consider the linear discrete ill-posed problem

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

where the norm $\|\cdot\|$ is the 2-norm of a vector or matrix, 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. (1.1) arises from many applications, e.g., from the discretization of the first kind Fredholm integral equation

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

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, groundwater modeling, and many others [1, 9, 10, 24, 35, 36, 37, 39, 47]. 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 $x_{naive} = A^\dagger b$ of (1.1) generally bears no relation to the true solution $x_{true} = A^\dagger b_{true}$, where \dagger denotes the Moore-Penrose inverse of

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a matrix. Therefore, we must use regularization to extract a good approximation to x_{true} as much as possible.

For a Gaussian white noise e , throughout the paper, we always assume that b_{true} satisfies the discrete Picard condition $\|A^\dagger b_{true}\| \leq C$ with some constant C for $\|A^\dagger\|$ arbitrarily large [1, 13, 20, 21, 22, 24, 36]. Without loss of generality, assume that $Ax_{true} = b_{true}$. Then a dominating regularization approach is to solve the problem

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

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} .

In this paper, we are concerned with the case $L = I$ in (1.3), which corresponds to a 2-norm filtering regularization problem. Let

$$(1.4) \quad A = U \begin{pmatrix} \Sigma \\ \mathbf{0} \end{pmatrix} V^T$$

be the singular value decomposition (SVD) of A , where $U = (u_1, u_2, \dots, u_m) \in \mathbb{R}^{m \times m}$ and $V = (v_1, v_2, \dots, v_n) \in \mathbb{R}^{n \times n}$ are orthogonal, $\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_n) \in \mathbb{R}^{n \times n}$ with the singular values $\sigma_1 > \sigma_2 > \dots > \sigma_n > 0$ assumed to be simple, the superscript T denotes the transpose of a matrix or vector, and $\mathbf{0}$ denotes a zero matrix. With (1.4), we have

$$(1.5) \quad x_{naive} = \sum_{i=1}^n \frac{u_i^T b}{\sigma_i} v_i = \sum_{i=1}^n \frac{u_i^T b_{true}}{\sigma_i} v_i + \sum_{i=1}^n \frac{u_i^T e}{\sigma_i} v_i = x_{true} + \sum_{i=1}^n \frac{u_i^T e}{\sigma_i} v_i$$

$$\text{and } \|x_{true}\| = \|A^\dagger b_{true}\| = \left(\sum_{i=1}^n \frac{|u_i^T b_{true}|^2}{\sigma_i^2} \right)^{1/2}.$$

The discrete Picard condition means that, on average, the Fourier coefficient $|u_i^T b_{true}|$ decays faster than σ_i , which results in the following popular model that is used throughout Hansen's books [22, 24] and the references therein as well as [32, 33]:

$$(1.6) \quad |u_i^T b_{true}| = \sigma_i^{1+\beta}, \quad \beta > 0, \quad i = 1, 2, \dots, n,$$

where β is a model parameter that controls the decay rates of $|u_i^T b_{true}|$.

The covariance matrix of the Gaussian white noise e is $\eta^2 I$, the expected value $\mathcal{E}(\|e\|^2) = m\eta^2$ and $\mathcal{E}(|u_i^T e|) = \eta$, $i = 1, 2, \dots, n$, so that $\|e\| \approx \sqrt{m}\eta$ and $|u_i^T e| \approx \eta$, $i = 1, 2, \dots, n$. (1.5) and (1.6) show that, for large singular values, $|u_i^T b_{true}|/\sigma_i$ is dominant relative to $|u_i^T e|/\sigma_i$. Once $|u_i^T b_{true}| \leq |u_i^T e|$ from some i onwards, the noise e dominates $|u_i^T b|$, and the terms $\frac{|u_i^T b|}{\sigma_i} \approx \frac{|u_i^T e|}{\sigma_i}$ overwhelm x_{true} for small singular values and must be dampened. Therefore, the transition point k_0 is such that

$$(1.7) \quad |u_{k_0}^T b| \approx |u_{k_0}^T b_{true}| > |u_{k_0}^T e| \approx \eta, \quad |u_{k_0+1}^T b| \approx |u_{k_0+1}^T e| \approx \eta;$$

see [24, p.42, 98] and [22, p.70-1].

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 a sequence of problems

$$(1.8) \quad \min \|x\| \quad \text{subject to} \quad \|A_k x - b\| = \min$$

starting with $k = 1$ onwards, 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 $U_k = (u_1, \dots, u_k)$, $V_k = (v_1, \dots, v_k)$ and $\Sigma_k =$

$\text{diag}(\sigma_1, \dots, \sigma_k)$; it holds that $\|A - A_k\| = \sigma_{k+1}$ [3, p.12], and $x_k^{tsvd} = A_k^\dagger b$ solves (1.8), called the TSVD regularized solution. For the Gaussian white noise e it is known from [22, p.70-1] and [24, p.71,86-8,95] that $x_{k_0}^{tsvd}$ is the 2-norm filtering best TSVD regularized solution of (1.1), i.e., $x_{k_0}^{tsvd}$ has the minimal 2-norm error $\|x_{true} - x_{k_0}^{tsvd}\| = \min_{k=1,2,\dots,n} \|x_{true} - x_k^{tsvd}\|$. The index k plays the role of the regularization parameter in the TSVD method. It has been observed and justified that $x_{k_0}^{tsvd}$ is essentially a 2-norm filtering best possible solution of (1.1); see [21], [22, p.109-11], [24, Sections 4.2 and 4.4] and [46]. We refer to [32] for general elaborations. As a result, we can take $x_{k_0}^{tsvd}$ as the standard reference when assessing the regularization ability of a 2-norm filtering regularization method.

For A large, the TSVD method is generally prohibitively expensive, and only iterative regularization methods are appealing. Krylov iterative solvers have formed a major class of methods [1, 10, 14, 17, 22, 24, 37]. Specifically, the CGLS method [15, 26] and its mathematically equivalent LSQR method [41], the CGME method [3, 4, 6, 17, 18] and the LSMR method [4, 5, 12] have been commonly used. These methods are deterministic 2-norm filtering regularization methods, 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 iterates first converge to x_{true} , then the noise e starts to deteriorate the iterates so that they start to diverge from x_{true} and instead converge to x_{naive} . The iteration number plays the role of the regularization parameter in iterative regularization methods.

The behavior of ill-posed problems and solvers depends on the decay rate of σ_j . Hoffmann [29] has characterized the degree of ill-posedness of (1.1) as follows: If $\sigma_j = \mathcal{O}(\rho^{-j})$ with $\rho > 1$, $j = 1, 2, \dots, n$, 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]. The requirement $\alpha > \frac{1}{2}$ does not appear in [29] and is explicitly added in [30, 32], which is always met for a linear compact operator equation [19, 22].

Hanke and Hansen [19] address that a strict proof of the regularizing properties of conjugate gradients is extremely difficult; see also [23]. The regularizing effects of CGLS, LSQR and CGME have been intensively studied; see, e.g., and have been intensively studied [1, 8, 11, 14, 17, 18, 22, 24, 27, 28, 30, 32, 33, 42, 45]. It has long been known (cf. [19, 22, 23, 24]) that if the singular values of the projection matrices involved in LSQR, called the Ritz values, approximate the large singular values in natural order then LSQR has the same regularization ability as the TSVD method, that is, the two methods can compute 2-norm filtering best 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 $A^T A$ in this order, respectively.

If a 2-norm filtering regularized solution of (1.1) is as accurate as $x_{k_0}^{tsvd}$, 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 [30, 32]. In terms of it, a fundamental question posed in [30, 32] is: *Do CGLS, LSQR, CGME and LSMR have the full or partial regularization for severely, moderately and mildly ill-posed problems?* Actually, this question has been receiving high attention for CGLS and LSQR.

For the cases that σ_i are simple, the author in [32] has given accurate estimates for the 2-norm distances between the underlying k dimensional Krylov subspace and the k

dimensional dominant right singular subspace $\text{span}\{V_k\}$ of A for severely, moderately and mildly ill-posed problems. On the basis of [32], the author in [33] has proved that, for LSQR, the k Ritz values converge to the k large singular values of A in natural order and Lanczos bidiagonalization always generates a near best rank k approximation until $k = k_0$ for severely and moderately ill-posed problems with suitable $\rho > 1$ and $\alpha > 1$, meaning that LSQR and CGLS have the full regularization. However, if such desired properties fail to hold, it has been theoretically unknown if LSQR has the full or partial regularization. Nevertheless, numerical experiments on many ill-posed problems have demonstrated that LSQR always has the full regularization [32, 33].

In this paper, we analyze the regularization of CGME and LSMR under the assumption that all the singular values σ_i are simple. We establish a number of results, and 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. Specifically, we derive the filtered SVD expansion of CGME iterates, by which we prove that the semi-convergence of CGME always occurs no later than that of LSQR and can be much earlier than the latter. In the meantime, we show how to extract a rank k approximation from the rank $k + 1$ approximation to A generated in CGME at iteration k , which is as accurate as the rank k approximation in LSQR. Exploiting such rank k approximation, we propose a modified CGME (MCGME) method whose regularization ability is shown to be very comparable to that of LSQR. For LSMR, we present a number of results and prove that its regularization ability is as good as that of LSQR and the two methods compute the 2-norm filtering best regularized solutions with essentially the same accuracy. We also show that the semi-convergence of LSMR always occurs no sooner than that of LSQR.

As a windfall, making 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 and have been used in numerous disciplines 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 for the approximation accuracy are not only unconditionally sharper than theirs but also can reveal how the truncation step damages the accuracy of the rank k approximation.

The paper is organized as follows. In Section 2, we review LSQR, CGME and LSMR. In Section 3, we briefly state some results on LSQR in [32, 33] and take LSQR as reference to assess the regularization ability of CGME and LSMR. In Section 4, we derive a number of regularization properties of CGME and propose the MCGME method. In Section 5, we consider the accuracy of the truncated rank k randomized approximation [16] and present sharper bounds. 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 $\mathcal{K}_k(C, w) = \text{span}\{w, Cw, \dots, C^{k-1}w\}$ the k dimensional Krylov subspace generated by the matrix C and the vector w , and by the bold letter $\mathbf{0}$ the zero matrix with orders clear from the context.

2. The LSQR, CGME and LSMR algorithms. These three algorithms are all based on the Lanczos bidiagonalization process, which computes two orthonormal bases $\{q_1, q_2, \dots, q_k\}$ and $\{p_1, p_2, \dots, p_{k+1}\}$ of $\mathcal{K}_k(A^T A, A^T b)$ and $\mathcal{K}_{k+1}(AA^T, b)$ for $k = 1, 2, \dots, n$, respectively. We describe the process as Algorithm 1.

Algorithm 1: k -step Lanczos bidiagonalization process

1. Take $p_1 = b/\|b\| \in \mathbb{R}^m$, and define $\beta_1 q_0 = \mathbf{0}$.
2. For $j = 1, 2, \dots, k$
 - (i) $r = A^T p_j - \beta_j q_{j-1}$
 - (ii) $\alpha_j = \|r\|; q_j = r/\alpha_j$
 - (iii) $z = A q_j - \alpha_j p_j$
 - (iv) $\beta_{j+1} = \|z\|; p_{j+1} = z/\beta_{j+1}$.

Algorithm 1 can be written in the matrix form

$$(2.1) \quad A Q_k = P_{k+1} B_k,$$

$$(2.2) \quad A^T P_{k+1} = Q_k B_k^T + \alpha_{k+1} q_{k+1} (e_{k+1}^{(k+1)})^T,$$

where $e_{k+1}^{(k+1)}$ denotes the $(k+1)$ -th canonical basis vector of \mathbb{R}^{k+1} , $P_{k+1} = (p_1, p_2, \dots, p_{k+1})$, $Q_k = (q_1, q_2, \dots, q_k)$ and

$$(2.3) \quad B_k = \begin{pmatrix} \alpha_1 & & & & & \\ \beta_2 & \alpha_2 & & & & \\ & \beta_3 & \ddots & & & \\ & & & \ddots & & \\ & & & & \alpha_k & \\ & & & & & \beta_{k+1} \end{pmatrix} \in \mathbb{R}^{(k+1) \times k}.$$

It is known from (2.1) that

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

Algorithm 1 cannot break down before step n when σ_i , $i = 1, 2, \dots, n$, are simple since b is supposed to have nonzero components in the directions of u_i , $i = 1, 2, \dots, n$. The singular values $\theta_i^{(k)}$, $i = 1, 2, \dots, k$ of B_k , called the Ritz values of A with respect to the left and right subspaces $\text{span}\{P_{k+1}\}$ and $\text{span}\{Q_k\}$, are all simple.

Write $\mathcal{V}_k^R = \mathcal{K}_k(A^T A, A^T b)$ and $\beta_1 = \|b\|$. At iteration k , LSQR [41] solves

$$\|A x_k^{lsqr} - b\| = \min_{x \in \mathcal{V}_k^R} \|A x - b\|$$

for the iterate

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

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

CGME [4, 17, 18, 27, 28] is the CG method implicitly applied to $\min \|A A^T y - b\|$ or $A A^T y = b$ with $x = A^T y$, and it solves the problem

$$\|x_{naive} - x_k^{cgme}\| = \min_{x \in \mathcal{V}_k^R} \|x_{naive} - x\|$$

for the iterate x_k^{cgme} . The error norm $\|x_{naive} - x_k^{cgme}\|$ 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.,

$$(2.6) \quad \bar{B}_k = P_k^T A Q_k.$$

Then the CGME iterate

$$(2.7) \quad x_k^{cgme} = Q_k y_k^{cgme} \quad \text{with} \quad y_k^{cgme} = \beta_1 \bar{B}_k^{-1} e_1^{(k)}$$

and $\|Ax_k^{cgme} - b\| = \beta_{k+1} |(e_k^{(k)})^T y_k^{cgme}|$ with $e_k^{(k)}$ the k -th canonical vector of \mathbb{R}^{k+1} .

LSMR [4, 12] is mathematically equivalent to MINRES [40] applied to the normal equation $A^T A x = A^T b$ of (1.1), and it solves

$$\|A^T(b - Ax_k^{lsmr})\| = \min_{x \in \mathcal{V}_k^R} \|A^T(b - Ax)\|$$

for the iterate x_k^{lsmr} . The residual norm $\|A^T(b - Ax_k^{lsmr})\|$ of the normal equation decreases monotonically with respect to k , and the iterate

$$(2.8) \quad x_k^{lsmr} = Q_k y_k^{lsmr} \quad \text{with} \quad y_k^{lsmr} = \arg \min_{y \in \mathbb{R}^k} \|(B_k^T B_k, \alpha_{k+1} \beta_{k+1} e_k^{(k)})^T y - \alpha_1 \beta_1 e_1^{(k+1)}\|.$$

3. Some results on LSQR in [32, 33]. From $\beta_1 e_1^{(k+1)} = P_{k+1}^T b$ and (2.5) we have

$$(3.1) \quad x_k^{lsqr} = Q_k B_k^\dagger P_{k+1}^T b,$$

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 $\|A - A_k\| = \sigma_{k+1}$. Analogous to (1.8), LSQR now solves a sequence of problems

$$(3.2) \quad \min \|x\| \quad \text{subject to} \quad \|P_{k+1} B_k Q_k^T x - b\| = \min$$

for x_k^{lsqr} starting with $k = 1$ onwards, where A in (1.1) is replaced by a rank k approximation $P_{k+1} B_k Q_k^T$ of it. Therefore, if $P_{k+1} B_k Q_k^T$ is a near best rank k approximation to A with an approximate accuracy σ_{k+1} and the singular values $\theta_i^{(k)}$, $i = 1, 2, \dots, k$ of B_k approximate the k large σ_i in natural order for $k = 1, 2, \dots, k_0$, then LSQR has the same regularization ability as the TSVD method and thus has the full regularization. See [32] for more elaborations.

The analysis on the TSVD method and the Tikhonov regularization method [22, 24] shows that the core requirement on a regularization method is to acquire the k_0 dominant SVD components of A and meanwhile suppress the remaining $n - k_0$ SVD components. Therefore, the more accurate the rank k approximation is to A and the better approximations are the k non-zero singular values of a projection matrix to some of the k_0 large singular values of A , the better regularization ability of the method has, so that the best regularized solution obtained by it is more accurate.

Define

$$(3.3) \quad \gamma_k^{lsqr} = \|A - P_{k+1} B_k Q_k^T\|,$$

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

$$\gamma_k^{lsqr} \geq \sigma_{k+1}.$$

The author in [33] introduces the definition of a near best rank k approximation to A : For LSQR, $P_{k+1} B_k Q_k^T$ is called a near best rank k approximation to A if γ_k^{lsqr} is closer to σ_{k+1} than to σ_k :

$$(3.4) \quad \sigma_{k+1} \leq \gamma_k^{lsqr} < \frac{\sigma_k + \sigma_{k+1}}{2}.$$

Based on the accurate estimates established in [32] for the 2-norm distances between the underlying Krylov subspace \mathcal{V}_k^R and the k dimensional dominant right singular subspace $span\{V_k\}$ for severely, moderately and mildly ill-posed problems, the author [33] has derived accurate estimates for γ_k^{lsqr} and a number of approximation properties of $\theta_i^{(k)}$, $i = 1, 2, \dots, k$ for the three kinds of ill-posed problems. The results have shown that, for severely and moderately ill-posed problems with for suitable $\rho > 1$ and $\alpha > 1$ and for $k = 1, 2, \dots, k_0$, $P_{k+1}B_kQ_k^T$ must be a near best rank k approximation to A , and the k Ritz values $\theta_i^{(k)}$ approximate the large singular values σ_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 $\alpha > 1$ not enough 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 for some $k \leq k^*$.

In particular, the author [33, Theorem 5.1] has proved the following three results:

$$(3.5) \quad \gamma_k^{lsqr} = \|G_k\|$$

with

$$(3.6) \quad G_k = \begin{pmatrix} \alpha_{k+1} & & & & & \\ \beta_{k+2} & \alpha_{k+2} & & & & \\ & \beta_{k+3} & \ddots & & & \\ & & & \ddots & & \\ & & & & \alpha_n & \\ & & & & & \beta_{n+1} \end{pmatrix} \in \mathbb{R}^{(n-k+1) \times (n-k)},$$

$$(3.7) \quad \alpha_{k+1} < \gamma_k^{lsqr}, \quad \beta_{k+2} < \gamma_k^{lsqr}, \quad k = 1, 2, \dots, n-1,$$

$$(3.8) \quad \gamma_{k+1}^{lsqr} < \gamma_k^{lsqr}, \quad k = 1, 2, \dots, n-2.$$

These notation and results will be used later.

4. The regularization of CGME. Note that $P_k^T b = \beta_1 e_1^{(k)}$. We obtain

$$(4.1) \quad x_k^{cgme} = Q_k \bar{B}_k^{-1} P_k^T b.$$

Therefore, analogous to (1.8) and (3.2), CGME solves a sequence of problems

$$(4.2) \quad \min \|x\| \quad \text{subject to} \quad \|P_k \bar{B}_k Q_k^T x - b\| = \min$$

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

Just as LSQR, if $P_k \bar{B}_k Q_k^T$ is a near best rank k approximation to A and the k singular values of \bar{B}_k approximate the large ones of A in natural order for $k = 1, 2, \dots, k_0$, then CGME has the full regularization.

By (2.1), (2.2) and (2.4), the rank k approximation involved in LSQR is

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

By (3.3), we have $\gamma_k^{lsqr} = \|A(I - Q_k Q_k^T)\|$. For CGME, by (2.2) and (2.6), we obtain

$$(4.4) \quad \begin{aligned} P_{k+1} P_{k+1}^T A &= P_{k+1} (B_k Q_k^T + \alpha_{k+1} e_{k+1}^{(k+1)} q_{k+1}^T) \\ &= P_{k+1} (B_k, \alpha_{k+1} e_{k+1}^{(k+1)}) Q_{k+1}^T \\ &= P_{k+1} \bar{B}_{k+1} Q_{k+1}^T. \end{aligned}$$

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

$$(4.5) \quad \gamma_k^{cgme} = \|A - P_k \bar{B}_k Q_k^T\| = \|(I - P_k P_k^T)A\|.$$

THEOREM 4.1. *For the rank k approximations $P_k P_k^T A = P_k \bar{B}_k Q_k^T$ to A , $k = 1, 2, \dots, n-1$, with the definition $\gamma_0^{lsqr} = \|A\|$ we have*

$$(4.6) \quad \gamma_k^{lsqr} < \gamma_k^{cgme} < \gamma_{k-1}^{lsqr},$$

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

Proof. We give two proofs of the upper bound in (4.6). The first is as follows. Since $P_{k+1} P_{k+1}^T (I - P_{k+1} P_{k+1}^T) = \mathbf{0}$, from (2.2) we obtain

$$\begin{aligned} (\gamma_k^{lsqr})^2 &= \|A - P_{k+1} B_k Q_k^T\|^2 \\ &= \|P_{k+1} P_{k+1}^T A - P_{k+1} B_k Q_k^T + (I - P_{k+1} P_{k+1}^T)A\|^2 \\ &= \max_{\|y\|=1} \|((P_{k+1} P_{k+1}^T A - P_{k+1} B_k Q_k^T) + (I - P_{k+1} P_{k+1}^T)A)y\|^2 \\ &= \max_{\|y\|=1} \|P_{k+1} P_{k+1}^T (P_{k+1} P_{k+1}^T A - P_{k+1} B_k Q_k^T)y + (I - P_{k+1} P_{k+1}^T)Ay\|^2 \\ &= \max_{\|y\|=1} (\|P_{k+1} P_{k+1}^T (P_{k+1} P_{k+1}^T A - P_{k+1} B_k Q_k^T)y\|^2 + \|(I - P_{k+1} P_{k+1}^T)Ay\|^2) \\ &= \max_{\|y\|=1} (\|P_{k+1} (P_{k+1}^T A - B_k Q_k^T)y\|^2 + \|(I - P_{k+1} P_{k+1}^T)Ay\|^2) \\ &= \max_{\|y\|=1} (\|(P_{k+1}^T A - B_k Q_k^T)y\|^2 + \|(I - P_{k+1} P_{k+1}^T)Ay\|^2) \\ &= \max_{\|y\|=1} (\alpha_{k+1}^2 |(e_{k+1}^{(k+1)})^T y|^2 + \|(I - P_{k+1} P_{k+1}^T)Ay\|^2) \\ &> \max_{\|y\|=1} \|(I - P_{k+1} P_{k+1}^T)Ay\|^2 \\ &= \|(I - P_{k+1} P_{k+1}^T)A\|^2 = (\gamma_{k+1}^{cgme})^2, \end{aligned}$$

which is the upper bound in (4.6) by replacing the index $k+1$ with k .

Taking $k = n$ in (2.4) and augmenting P_{n+1} such that $P = (P_{n+1}, \hat{P}) \in \mathbb{R}^{m \times m}$ is orthogonal, we have

$$(4.8) \quad P^T A Q_n = \begin{pmatrix} B_n \\ \mathbf{0} \end{pmatrix},$$

where all the entries α_i and β_{i+1} , $i = 1, 2, \dots, n$, 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

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

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 $(\beta_k e_1, G_k) \in \mathbb{R}^{(n-k+1) \times (n-k+1)}$ 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 also give the second proof of the upper bound in (4.6). Observe from (3.6) that $(\beta_{k+1} e_1, G_k)$ is the matrix 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 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). \square

(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 $A Q_k Q_k^T = P_{k+1} B_k Q_k^T$ in LSQR. (4.7) shows the strict monotonic decreasing property of γ_k^{cgme} . Moreover, keep in mind that $\gamma_k^{lsqr} \geq \sigma_{k+1}$. Then a combination of it and the results in Section 3 indicates that, unlike $P_{k+1} B_k Q_k^T$ in LSQR, there is no guarantee that $P_k \bar{B}_k Q_k^T$ is a near best rank k approximation to A even for severely and moderately ill-posed problems, because γ_k^{cgme} simply lies between γ_k^{lsqr} and γ_{k-1}^{lsqr} and there do not exist any sufficient conditions on $\rho > 1$ and $\alpha > 1$ that enforce γ_k^{cgme} to be closer to γ_k^{lsqr} , let alone closer to σ_{k+1} . Therefore, based on the accuracy of the rank k approximations in CGME and LSQR, we come to the conclusion that the regularization ability of CGME cannot be superior and is generally inferior to that of LSQR. Furthermore, since there is no guarantee that $P_k \bar{B}_k Q_k^T$ is a near best rank k approximation for severely and moderately ill-posed problems with suitable $\rho > 1$ and $\alpha > 1$, CGME may not have the full regularization for these two kinds of problems.

In the following we investigate the approximation behavior of the k singular values $\bar{\theta}_i^{(k)}$ of \bar{B}_k , $k = 1, 2, \dots, n$. Before proceeding, it is necessary to have a closer look at Algorithm 1 and distinguish some subtleties when A is rectangular, i.e., $m > n$, and square, i.e., $m = n$, respectively.

Keep in mind that Algorithm 1 does not break down before step n . For the rectangular case $m > n$, Algorithm 1 is exactly what is presented there, all the α_k and β_{k+1} are positive, $k = 1, 2, \dots, n$, and we generate P_{n+1} and Q_n at step n and $\alpha_{n+1} = \beta_{n+2} = 0$. As a consequence, by definition (4.4), we have

$$(4.10) \quad \bar{B}_{n+1} = (B_n, \alpha_{n+1} e_{n+1}^{(n+1)}) = (B_n, \mathbf{0}).$$

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

For the square case $m = n$, 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} , which is impossible since P_n is already an orthogonal matrix. After Algorithm 1 is run to completion, we have

$$\bar{B}_n = P_n^T A Q_n,$$

whose singular values $\bar{\theta}_i^{(n)} = \sigma_i$, $i = 1, 2, \dots, n$.

By the definition (4.4) of \bar{B}_k , from (2.2) and the above description, for both the rectangular and square cases we obtain

$$(4.11) \quad P_k^T A A^T P_k = \bar{B}_k \bar{B}_k^T, \quad k = 1, 2, \dots, n^*,$$

with $n^* = n+1$ for $m > n$ and $n^* = n$ for $m = n$, which are unreduced symmetric tridiagonal matrices. For $m = n$, the eigenvalues of $A A^T$ are just σ_i^2 , $i = 1, 2, \dots, n$,

all of which are simple and positive; for $m > n$, the eigenvalues of AA^T are σ_i^2 , $i = 1, 2, \dots, n$ plus $m - n$ zeros, denoted by $\sigma_{n+1}^2 = \dots = \sigma_m^2 = 0$ for our later use. Therefore, by the definition of n^* , the eigenvalues of $\bar{B}_{n^*} \bar{B}_{n^*}^T$ are σ_i^2 , $i = 1, 2, \dots, n^*$.

Notice that $\bar{B}_k \bar{B}_k^T$ is nothing but the projection matrix of AA^T onto the k dimensional Krylov subspace $\mathcal{K}_k(AA^T, b)$. More precisely, $\bar{B}_k \bar{B}_k^T$ is generated by the k -step symmetric Lanczos tridiagonalization process applied to AA^T starting with $p_1 = b/\|b\|$, and the eigenvalues of $\bar{B}_k \bar{B}_k^T$ generally approximate extreme eigenvalues of AA^T ; see, e.g., [3, 4, 43] for details. Particularly, the smallest eigenvalue $(\bar{\theta}_k^{(k)})^2$ of $\bar{B}_k \bar{B}_k^T$ generally converges to the smallest eigenvalue $\sigma_{n^*}^2$ of AA^T as k increases, which is $\sigma_{n+1}^2 = 0$ for $m > n$ and $\sigma_n^2 > 0$ for $m = n$. In contrast, for B_k , its smallest singular value $\theta_k^{(k)} > \sigma_n$ unconditionally until $\theta_n^{(n)} = \sigma_n$.

We next give a number of close relationships between $\bar{\theta}_i^{(k)}$ and $\theta_i^{(k)}$ as well as between them and the singular values σ_i of A , which are crucial to compare the regularizing effects of CGME with those of LSQR.

THEOREM 4.2. *Denote by $\bar{\theta}_i^{(k)}$ and $\theta_i^{(k)}$, $i = 1, 2, \dots, k$ the singular values of \bar{B}_k and B_k , respectively, labeled in decreasing order. Then*

$$(4.12) \quad \theta_1^{(k)} > \bar{\theta}_1^{(k)} > \theta_2^{(k)} > \bar{\theta}_2^{(k)} > \dots > \theta_k^{(k)} > \bar{\theta}_k^{(k)}, \quad k = 1, 2, \dots, n-1.$$

Moreover,

$$(4.13) \quad \sigma_n < \bar{\theta}_k^{(k)} < \theta_k^{(k)} < \sigma_k, \quad k = 1, 2, \dots, n-1$$

for $m = n$ and

$$(4.14) \quad \sigma_n < \theta_k^{(k)} < \sigma_k, \quad k = 1, 2, \dots, n-1,$$

$$(4.15) \quad 0 < \bar{\theta}_k^{(k)} < \theta_k^{(k)} < \sigma_k, \quad k = 1, 2, \dots, n-1$$

for $m > n$.

Proof. Observe that \bar{B}_k consists of the first k rows of B_k and all the α_k and β_{k+1} are positive for $k = 1, 2, \dots, n-1$. Applying the strict interlacing property of singular values to \bar{B}_k and B_k , we obtain (4.12).

Note that, for A both rectangular and square, we have $\theta_i^{(n)} = \sigma_i$, $i = 1, 2, \dots, n$. 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 (cf. [44, p.198, Corollary 4.4]), for $k = 1, 2, \dots, n-1$ we have

$$(4.16) \quad \sigma_{n-k+i} < \theta_i^{(k)} < \sigma_i, \quad i = 1, 2, \dots, k.$$

Observe that $\bar{B}_k \bar{B}_k^T$, $k = 1, 2, \dots, n-1$, are the $k \times k$ leading principal matrices of $\bar{B}_{n^*} \bar{B}_{n^*}^T$, whose eigenvalues are σ_i^2 , $i = 1, 2, \dots, n^*$, and they are unreduced symmetric tridiagonal matrices. Applying the strict interlacing property of eigenvalues to $\bar{B}_k \bar{B}_k^T$ and $\bar{B}_{n^*} \bar{B}_{n^*}^T$, for $k = 1, 2, \dots, n-1$ we obtain

$$\sigma_{n^*-k+i}^2 < (\bar{\theta}_i^{(k)})^2 < \sigma_i^2, \quad i = 1, 2, \dots, k,$$

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). \square

From Section 3, (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 σ_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 σ_{k+1} and it can be as small as σ_n for $m = n$ and arbitrarily small for $m > n$, independent of ρ or α . In other words, the size of ρ or α has no intrinsic effects on the size of $\bar{\theta}_k^{(k)}$, and cannot make $\bar{\theta}_k^{(k)}$ lie between σ_{k+1} and σ_k by choosing ρ or α , that is, the regularizing effects of CGME have intrinsic indeterminacy for severely and moderately ill-posed problems, independent of the size of ρ and α . Therefore, CGME may or may not have the full regularization for these two kinds of problems. On the other hand, even if the $\bar{\theta}_i^{(k)}$ approximate the first k large singular values σ_i in natural order, they are less accurate than the k singular values $\theta_i^{(k)}$ of B_k because of (4.13) and (4.15). Consequently, since the $\theta_i^{(k)}$ are always correspondingly larger than the $\bar{\theta}_i^{(k)}$, the regularization ability of CGME cannot be superior and is generally 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 $\bar{\theta}_k^{(k)}$ converges to zero other than σ_n as k increases and can be arbitrarily small, which causes that the projected problem $\bar{B}_k y_k^{cgme} = \beta_1 e_1^{(k)}$ may even be worse conditioned than (1.1) and $\|x_k^{cgme}\| = \|y_k^{cgme}\|$ may be unbounded as k increases and bigger than $\|x_{naive}\|$ for a given (1.1).

In what follows we establish more results on the regularization of CGME and get more insight into it. It is known, e.g., [22, p.146] that the LSQR iterate x_k^{lsqr} takes the following filtered SVD expansion:

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

where the filters

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

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 iterate x_k^{cgme} also takes a filtered SVD expansion similar to (4.17) and (4.18), but its proof is much more involved than that of (4.17) and (4.18).

THEOREM 4.3. *The CGME iterate x_k^{cgme} has the filtered SVD expansion*

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

where the filters

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

Proof. Let $y_{naive} = (AA^T)^\dagger b$ be the minimal 2-norm solution to $\min_y \|AA^T y - b\|$. Recall Algorithm 1. For this minimization problem, starting with $y_0^{cgme} = \mathbf{0}$, at iteration k the CG method extracts y_k^{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^{cgme} is

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

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 $(\bar{\theta}_j^{(k)})^2$ of AA^T with respect to the subspace $\text{span}\{P_k\}$; see (4.11). Therefore, we have

$$(4.22) \quad r_k(\sigma_i^2) = \prod_{j=1}^n \frac{(\bar{\theta}_j^{(k)})^2 - \sigma_i^2}{(\bar{\theta}_j^{(k)})^2}, \quad i = 1, 2, \dots, n.$$

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

$$\begin{aligned} y_{naive} - U_n U_n^T y_k^{cgme} &= (AA^T)^\dagger r_k(AA^T)b \\ &= r_k(AA^T)(AA^T)^\dagger b = r_k(AA^T)y_{naive}, \end{aligned}$$

from which it follows that

$$(4.23) \quad U_n U_n^T y_k^{cgme} = (I - r_k(AA^T))y_{naive}.$$

By the SVD (1.4) of A , we have

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

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

$$(4.24) \quad \begin{aligned} U_n U_n^T y_k^{cgme} &= \sum_{i=1}^n (1 - r_k(\sigma_i^2)) \frac{u_i^T b}{\sigma_i^2} u_i \\ &= \sum_{i=1}^n f_i^{(k, cgme)} \frac{u_i^T b}{\sigma_i^2} u_i \end{aligned}$$

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 hand 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). \square

Based on Theorems 4.2–4.3, we can prove the following important result.

THEOREM 4.4. *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*

$$(4.25) \quad k_{cgme}^* \leq k_{lsqr}^* \leq k_0,$$

that is, the semi-convergence of CGME always occurs no later than that of LSQR and the TSVD method.

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

$$x_{k_0}^{tsvd} = A_{k_0}^\dagger b = \sum_{i=1}^{k_0} \frac{u_i^T b}{\sigma_i} v_i$$

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 σ_i in natural order for $k = 1, 2, \dots, k_0$, then by (4.20) we have $f_i^{(k, cgme)} \rightarrow 1$ for $i = 1, 2, \dots, k$ and $f_i^{(k, cgme)} \rightarrow 0$ for $i = k + 1, \dots, n$. On the other hand, by (4.20) we have $f_{k_0+1}^{(k_0+1, cgme)} = \mathcal{O}(1)$. Compared with the best TSVD solution, by (4.19) the above shows that the CGME iterate x_k^{cgme} captures the k dominant SVD components of A and filters out the $n - k$ small ones. As a result, x_k^{cgme} improves until iteration k_0 , and the semi-convergence of CGME occurs at iteration $k_{cgme}^* = k_0$.

If the $\bar{\theta}_j^{(k)}$ do 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^{cgme} 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 $i = j^*, j^* + 1, \dots, n$, but

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

since the first factor is non-positive and the second factor is positive by noting that $\bar{\theta}_j^{(k)} > \sigma_i$, $j = 1, 2, \dots, k - 1$ for $i = k_0 + 1, \dots, j^* - 1$. As a result, $f_i^{(k, cgme)} \geq 1$ for $i = k_0 + 1, \dots, j^* - 1$, showing that x_k^{cgme} 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 $\bar{\theta}_k^{(k)} < \theta_k^{(k)}$ 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, applying a similar proof to that of the semi-convergence of CGME to (4.17)–(4.18), it is direct that the semi-convergence of CGME occurs no later than that of LSQR, i.e., $k_{cgme}^* \leq k_{lsqr}^*$. \square

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

$$(4.26) \quad \|x_{naive} - x_k^{cgme}\| \leq \|x_{naive} - x_k^{lsqr}\|$$

holds unconditionally for $i = 1, 2, \dots, n$. Since x_k^{cgme} and x_k^{lsqr} converge to x_{true} until iterations k_{cgme}^* and k_{lsqr}^* at which the semi-convergence of CGME and LSQR occurs, respectively, it is known that, for $k \leq k_{cgme}^*$ and $k \leq k_{lsqr}^*$, $\|x_{true} - x_k^{cgme}\|$ and $\|x_{true} - x_k^{lsqr}\|$ 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

$$(4.27) \quad \begin{aligned} \|x_{naive} - x_k^{cgme}\| &= \|x_{naive} - x_{true} + x_{true} - x_k^{cgme}\| \\ &\approx \|x_{naive} - x_{true}\| + \|x_{true} - x_k^{cgme}\|, \end{aligned}$$

$$(4.28) \quad \begin{aligned} \|x_{naive} - x_k^{lsqr}\| &= \|x_{naive} - x_{true} + x_{true} - x_k^{lsqr}\| \\ &\approx \|x_{naive} - x_{true}\| + \|x_{true} - x_k^{lsqr}\|. \end{aligned}$$

Since the first terms in the right-hand sides of (4.27) and (4.28) are the same constant, a combination of (4.26) with (4.27) and (4.28) means that

$$(4.29) \quad \|x_{true} - x_k^{cgme}\| \leq \|x_{true} - x_k^{lsqr}\|$$

generally holds until $k = k_{cgme}^*$. That is, x_k^{cgme} should be *at least* as accurate as x_k^{lsqr} until the semi-convergence of CGME occurs. Then for $k > k_{cgme}^*$, according to Theorem 4.4, x_k^{lsqr} continues approximating x_{true} as k increases until iteration $k = k_{lsqr}^*$, at which LSQR ultimately computes a more accurate approximation $x_{k_{lsqr}^*}^{lsqr}$ to x_{true} than $x_{k_{cgme}^*}^{cgme}$.

We will have more exciting findings. Observe that after Lanczos bidiagonalization is run k steps, we have already obtained \bar{B}_{k+1} , P_{k+1} and Q_{k+1} , but LSQR and CGME exploit only B_k , Q_k and \bar{B}_k , Q_k , respectively. Since $\alpha_{k+1} > 0$ for $k \leq n-1$, applying the strict interlacing property of singular values to B_k and \bar{B}_{k+1} , we have

$$(4.30) \quad \bar{\theta}_1^{(k+1)} > \theta_1^{(k)} > \bar{\theta}_2^{(k+1)} > \dots > \bar{\theta}_k^{(k+1)} > \theta_k^{(k)} > \bar{\theta}_{k+1}^{(k+1)}, \quad k = 1, 2, \dots, n-1.$$

Note from (4.15) that $\bar{\theta}_i^{(k+1)} < \sigma_i$, $i = 1, 2, \dots, k+1$. Combining (4.30) with (4.15), we see that as approximations to the first large k singular values σ_i of A , although the k singular values $\bar{\theta}_i^{(k)}$ of \bar{B}_k are less accurate than the singular values $\theta_i^{(k)}$ of B_k , the first k singular values $\bar{\theta}_i^{(k+1)}$ of \bar{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 $P_{k+1}\bar{B}_{k+1}Q_{k+1}^T = P_{k+1}P_{k+1}^T A$ generated by Algorithm 1.

THEOREM 4.5. *Let \bar{C}_k be the best rank k approximation to \bar{B}_{k+1} with respect to the 2-norm. Then for $k = 1, 2, \dots, n-1$ we have*

$$(4.31) \quad \|A - P_{k+1}\bar{C}_k Q_{k+1}^T\| \leq \sigma_{k+1} + \gamma_{k+1}^{cgme},$$

$$(4.32) \quad \|A - P_{k+1}\bar{C}_k Q_{k+1}^T\| \leq \bar{\theta}_{k+1}^{(k+1)} + \gamma_{k+1}^{cgme},$$

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

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

(4.33)

$$\begin{aligned} \|A - P_{k+1}\bar{C}_k Q_{k+1}^T\| &\leq \|A - P_{k+1}\bar{B}_{k+1}Q_{k+1}^T\| + \|P_{k+1}(\bar{B}_{k+1} - \bar{C}_k)Q_{k+1}^T\| \\ (4.34) \qquad \qquad \qquad &= \|A - P_{k+1}\bar{B}_{k+1}Q_{k+1}^T\| + \|P_{k+1}P_{k+1}^T A - P_{k+1}\bar{C}_k Q_{k+1}^T\|. \end{aligned}$$

By the definition of C_k and (4.4), it is easily justified that $P_{k+1}\bar{C}_k Q_{k+1}^T$ is the best rank k approximation to $P_{k+1}\bar{B}_{k+1}Q_{k+1}^T = P_{k+1}P_{k+1}^T A$ in the 2-norm as P_{k+1} and Q_{k+1} are column orthonormal. Keep in mind that A_k is the best rank k approximation to A . Since $P_{k+1}P_{k+1}^T A_k$ is a rank k approximation to $P_{k+1}P_{k+1}^T A$, we obtain

$$\begin{aligned} \|P_{k+1}P_{k+1}^T A - P_{k+1}\bar{C}_k Q_{k+1}^T\| &\leq \|P_{k+1}P_{k+1}^T A - P_{k+1}P_{k+1}^T A_k\| \\ &= \|P_{k+1}P_{k+1}^T (A - A_k)\| \\ &\leq \|A - A_k\| = \sigma_{k+1}. \end{aligned}$$

Note that the first term in the right-hand side of (4.34) is just γ_{k+1}^{cgme} . Therefore, it follows from (4.34) that (4.31) holds.

Since P_{k+1} and Q_{k+1} are column orthonormal and C_k is the best rank k approximation to \bar{B}_{k+1} , by the orthogonal invariance of 2-norm we obtain

$$\|P_{k+1}(\bar{B}_{k+1} - \bar{C}_k)Q_{k+1}^T\| = \|\bar{B}_{k+1} - \bar{C}_k\| = \bar{\theta}_{k+1}^{(k+1)},$$

which, together with (4.33), yields (4.32). \square

The bound (4.32) is always smaller than the bound (4.31) because of $\bar{\theta}_{k+1}^{(k+1)} < \sigma_{k+1}$ from (4.13) and (4.15). Indeed, the bound (4.31) can be conservative since we have amplified $\|P_{k+1}(\bar{B}_{k+1} - \bar{C}_k)Q_{k+1}^T\|$ twice and obtained its bound σ_{k+1} , which might be a considerable overestimate. Moreover, as we have explained previously, (4.13) and (4.15) show that $\bar{\theta}_{k+1}^{(k+1)} > \sigma_n$ may approach σ_n for $m = n$ and $\bar{\theta}_{k+1}^{(k+1)} > 0$ can be close to zero arbitrarily for $m > n$. By definition (3.3) of γ_k^{lsqr} , since $\gamma_{k+1}^{cgme} < \gamma_k^{lsqr}$ (cf. the upper bound of (4.6)), $\gamma_k^{lsqr} \geq \sigma_{k+1} > \bar{\theta}_{k+1}^{(k+1)}$ and $\|A - P_{k+1}\bar{C}_k Q_{k+1}^T\| \geq \sigma_{k+1}$, the right-hand side of (4.32) satisfies

$$\sigma_{k+1} \leq \bar{\theta}_{k+1}^{(k+1)} + \gamma_{k+1}^{cgme} < 2\gamma_k^{lsqr}.$$

Therefore, $\bar{\theta}_{k+1}^{(k+1)} + \gamma_{k+1}^{cgme}$ is as small as and can even be smaller than γ_k^{lsqr} , meaning that $P_{k+1}\bar{C}_k Q_{k+1}^T$ is as accurate as the rank k approximation $P_{k+1}B_k Q_k^T$ in LSQR.

Define $Q_{n+1} = (Q_n, \mathbf{0}) \in \mathbb{R}^{n \times (n+1)}$, and note from (4.10) that $\bar{B}_{n+1} = (B_n, \mathbf{0})$. Recall that the singular values of \bar{B}_{n+1} and B_n are $\bar{\theta}_i^{(n+1)}$, $i = 1, 2, \dots, n+1$ and $\theta_i^{(n)}$, $i = 1, 2, \dots, n$, respectively, and $\bar{\theta}_i^{(n+1)} = \theta_i^{(n)} = \sigma_i$, $i = 1, 2, \dots, n$ and $\bar{\theta}_{n+1}^{(n+1)} = 0$. From (4.8) and the definition of \bar{C}_n , since \bar{B}_{n+1} is of rank n , we have

$$\bar{C}_n = \bar{B}_{n+1}$$

and

$$A = P_{n+1}B_n Q_n^T = P_{n+1}\bar{B}_{n+1}Q_{n+1}^T = P_{n+1}\bar{C}_n Q_{n+1}^T.$$

Based on Theorem 4.5 and the analysis followed, just as done in CGME and LSQR, we can replace A in (1.1) by the rank k approximation $P_{k+1}\bar{C}_kQ_{k+1}^T$ and propose a modified CGME (MCGME) method that solves

$$(4.35) \quad \min \|x\| \quad \text{subject to} \quad \|P_{k+1}\bar{C}_kQ_{k+1}^T x - b\| = \min$$

for the regularized solution $x_k^{mcgme} = Q_{k+1}y_k^{mcgme}$ of (1.1) with

$$(4.36) \quad y_k^{mcgme} = \bar{C}_k^\dagger P_{k+1}^T b = \beta_1 \bar{C}_k^\dagger e_1^{(k+1)}$$

starting with $k = 1$ onwards. MCGME is expected to have the same regularization ability as LSQR because (i) the k nonzero singular values $\bar{\theta}_i^{(k+1)}$ of \bar{C}_k are more accurate than the k singular values $\theta_i^{(k)}$ of B_k as approximations to the first k singular values of A and (ii) $P_{k+1}\bar{C}_kQ_{k+1}^T$ is a rank k approximation which is as accurate as $P_{k+1}B_kQ_k^T$ in LSQR. Regarding implementations, we comment that the singular values, and left and right singular vectors of \bar{C}_k^\dagger is already available when \bar{C}_k is extracted from the SVD of \bar{B}_{k+1} , whose computational cost is $\mathcal{O}(k^3)$ flops. As a result, by (4.36) we can compute y_k^{mcgme} at cost of $\mathcal{O}(k^2)$ flops. A difference from CGME and LSQR is that MCGME seeks x_k^{mcgme} in the $k + 1$ dimensional Krylov subspace $\mathcal{K}_{k+1}(A^T A, A^T b)$ other than in $\mathcal{K}_k(A^T A, A^T b)$. Numerical experiments will justify that MCGME has very comparable regularizing effects to LSQR and can obtain the best regularized solutions with very similar accuracy to those by LSQR. We will not consider the by-product MCGME method further in this paper.

\bar{C}_k may have some other potential applications. For example, when we are required to compute several largest singular triplets of a large scale matrix A , we can use the nonzero singular values of \bar{C}_k to replace the ones of B_k as more accurate approximations to the largest singular values of A in Lanczos bidiagonalization type algorithms [34]. In such a way, exploiting the SVD of \bar{C}_k , we can also compute more accurate approximate left and right singular vectors of A simultaneously. A development of such modified algorithms is beyond the scope of this paper.

5. The accuracy of truncated rank k approximate SVDs by randomized algorithms. In this section, we deviate from the context of Krylov solvers. Using the analysis approach in the last section, we 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 $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_{\min\{m,n\}}$.

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 Ω .
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 ℓ SVD approximation $PP^T A = \hat{U} \tilde{\Sigma} \tilde{V}^T$ to A .
4. Let $B_{(k)} = \tilde{U}_k \tilde{\Sigma}_{(k)} \tilde{V}_k^T$ be the best rank k approximation to B with the diagonal $\tilde{\Sigma}_{(k)}$ being the first k diagonals of $\tilde{\Sigma}$, and \tilde{U}_k and \tilde{V}_k the first k columns of \tilde{U} and \tilde{V} , respectively. Form a truncated rank k SVD approximation $A_{(k)} = PB_{(k)} = \hat{U}_k \tilde{\Sigma}_{(k)} \tilde{V}_k^T$ to A with $\hat{U}_k = P \tilde{U}_k$.

For the approximation accuracy of $A_{(k)}$ to A , Halko *et al.* [16] establish a fundamental result (cf. Theorem 9.3 there):

$$(5.1) \quad \|A - A_{(k)}\| \leq \sigma_{k+1} + \|(I - PP^T)A\|.$$

Assume that the oversampling parameter $p \geq 4$. Making use of the probability theory, in terms of σ_{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 σ_{k+1} in (5.1) is generally conservative and an overestimate.

Motivated by the proof of (4.32) in Theorem 4.5, we can improve (5.1) substantially and reveal why (5.1) is an overestimate. Let

$$(5.2) \quad \tilde{\sigma}_1 \geq \tilde{\sigma}_2 \geq \cdots \geq \tilde{\sigma}_{k+p}$$

be the singular values of $B = P^T A$ defined in Algorithm 2. It is clear from Algorithm 2 that

$$P^T AA^T P = BB^T$$

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 $P = (p_1, p_2, \dots, p_{k+p})$, whose eigenvalues are $\tilde{\sigma}_i^2$, $i = 1, 2, \dots, k+p$. Keep in mind that the eigenvalues of AA^T are σ_i^2 , $i = 1, 2, \dots, \min\{m, n\}$ and $m - \min\{m, n\}$ zeros, denoted by $\sigma_{\min\{m, n\}+1}^2 = \cdots = \sigma_m^2 = 0$ for later use.

THEOREM 5.1. *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*

$$(5.3) \quad \|A - A_{(k)}\| \leq \tilde{\sigma}_{k+1} + \|(I - PP^T)A\|$$

with

$$(5.4) \quad \sigma_{m-p+1} \leq \tilde{\sigma}_{k+1} \leq \sigma_{k+1}.$$

Proof. Since P is orthonormal, the eigenvalues of BB^T interlace those of AA^T and satisfy (cf. [44, p.198, Corollary 4.4])

$$\sigma_{m-(k+p)+i} \leq \tilde{\sigma}_i \leq \sigma_i, \quad i = 1, 2, \dots, k+p,$$

from which (5.4) follows.

From Algorithm 2, we can write

$$\begin{aligned} A - A_{(k)} &= A - PP^T A + PP^T A - A_{(k)} \\ &= A - PP^T A + P\tilde{U}\tilde{\Sigma}\tilde{V}^T - P\tilde{U}_k\tilde{\Sigma}_{(k)}\tilde{V}_{(k)}^T \\ &= (I - PP^T)A + P(\tilde{U}\tilde{\Sigma}\tilde{V}^T - \tilde{U}_k\tilde{\Sigma}_{(k)}\tilde{V}_{(k)}^T). \end{aligned}$$

Since $B_{(k)}$ is the best rank k approximation to B , by the column orthonormality of P we obtain

$$\begin{aligned} \|A - A_{(k)}\| &\leq \|(I - PP^T)A\| + \|P(\tilde{U}\tilde{\Sigma}\tilde{V}^T - \tilde{U}_k\tilde{\Sigma}_{(k)}\tilde{V}_{(k)}^T)\| \\ &= \|(I - PP^T)A\| + \|\tilde{U}\tilde{\Sigma}\tilde{V}^T - \tilde{U}_k\tilde{\Sigma}_{(k)}\tilde{V}_{(k)}^T\| \\ &= \|(I - PP^T)A\| + \|B - B_{(k)}\| \\ &= \|(I - PP^T)A\| + \tilde{\sigma}_{k+1}, \end{aligned}$$

which proves (5.3). \square

REMARK 5.1. *This theorem indicates that $\tilde{\sigma}_{k+1}$ never exceeds σ_{k+1} and, for m, n large and $k + p$ small, it may be much smaller than σ_{k+1} . Specifically, $\tilde{\sigma}_{k+1}$ can be as small as σ_{m-p+1} . For $m > n$, whenever $m - p + 1 > n$, we have $\sigma_{m-p+1} = 0$. Consequently, the bound (5.3) is unconditionally superior to the bound (5.1) and is sharper than the latter when $\tilde{\sigma}_{k+1} < \sigma_{k+1}$. On the other hand, however, 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 the bound (5.3). Summarizing the above, in response of Remark 9.1 in [16], we conclude that 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 $\|(I - PP^T)A\| \geq \sigma_{k+1}$.*

As we have seen, the column space of P constructed by Algorithm 2 aims to capture the $(k + p)$ -dimensional dominant left singular subspace of A . A variant of it is to capture the $(k + p)$ -dimensional right dominant singular subspace of A . Mathematically, 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, for which (5.1) now becomes

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

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

Note that the eigenvalues of $A^T A$ are σ_i^2 , $i = 1, 2, \dots, \min\{m, n\}$ and $n - \min\{m, n\}$ zeros, denoted by $\sigma_{\min\{m, n\}+1}^2 = \dots = \sigma_n^2 = 0$. Since the eigenvalues of $(AP)^T AP$ interlace those of $A^T A$, using the same proof approach as that of Theorem 5.1, we can establish the following result.

THEOREM 5.2. *For $A \in \mathbb{R}^{m \times n}$, let P and $A_{(k)}$ be defined as in Algorithm 3, and $\tilde{\sigma}_1 \geq \tilde{\sigma}_2 \geq \dots \geq \tilde{\sigma}_{k+p}$ be the singular values of AP . Then*

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

with

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

We comment that, in the case $m < n$, whenever $n-p+1 > m$, we have $\sigma_{n-p+1} = 0$, and consequently the bound (5.6) is unconditionally superior to and can be substantially sharper than the bound (5.5) for m, n large and $k+p$ small.

REMARK 5.2. *If the singular values σ_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 5.3. (5.1) and (5.5) and Theorems 5.1–5.2 hold for all the truncated rank k SVD approximations generated by the enhanced variants of Algorithm 2–3 in [16], where the unique difference between the variants is the way that P is generated. More generally, Theorems 5.1–5.2 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 of LSMR. From Algorithm 1 we obtain

$$(6.1) \quad Q_{k+1}^T A^T A Q_k = (B_k^T B_k, \alpha_{k+1} \beta_{k+1} e_k^{(k)})^T.$$

Therefore, from (2.8), noting that $Q_{k+1}^T A^T b = \alpha_1 \beta_1 e_1^{(k+1)}$, we have

$$(6.2) \quad x_k^{lsmr} = Q_k (Q_{k+1}^T A^T A Q_k)^\dagger Q_{k+1}^T A^T b,$$

which means that LSMR solves the problem

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

for the regularized solution x_k^{lsmr} starting with $k = 1$ onwards. In the meantime, it is direct to justify that the TSVD solution x_k^{tsvd} solves the problem

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

starting with $k = 1$ onwards. Therefore, (6.3) and (6.4) deal with the normal equation $A^T A x = A^T b$ of (1.1) by replacing $A^T A$ with its rank k approximations $Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T$ and $A_k^T A_k$, respectively.

In view of (6.3) and (6.4), we need to accurately estimate the approximation accuracy $\|A^T A - Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T\|$ and investigate how the singular values of $Q_{k+1}^T A^T A Q_k$ approximate the k large singular values σ_i^2 , $i = 1, 2, \dots, k$ 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), (2.1), (2.2), (2.4) and $P_{k+1} P_{k+1}^T b = b$, the LSQR iterate

$$\begin{aligned} x_k^{lsqr} &= Q_k B_k^\dagger P_{k+1}^T b = Q_k (B_k^T B_k)^{-1} B_k^T P_{k+1}^T b \\ &= Q_k (Q_k^T A^T A Q_k)^{-1} Q_k^T A^T P_{k+1} P_{k+1}^T b \\ &= Q_k (Q_k^T A^T A Q_k)^{-1} Q_k^T A^T b, \end{aligned}$$

which is the solution to the problem

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

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.

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 $F_k^T F_k$ and zero. As a result, the eigenvalues of $F_k F_k^T$ are all simple. According to [7, p.218], we know from (6.11) 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 (6.10), establishes (6.6). \square

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

Recall that (3.3) measures the quality of the rank k approximation involved in LSQR for the regularization problem (3.2). We now estimate the approximation accuracy of $Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T$ to $A^T A$ in terms of $(\gamma_k^{lsqr})^2$.

THEOREM 6.2. *For $k = 1, 2, 3, \dots, n-1$, let γ_k^{lsqr} be defined as (3.3). For $k = 2, 3, \dots, n-1$ we have*

$$(6.13) \quad (\gamma_k^{lsqr})^2 < \|A^T A - Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T\| \leq \sqrt{1 + m_k (\gamma_{k-1}^{lsqr} / \gamma_k^{lsqr})^2} (\gamma_k^{lsqr})^2$$

with $0 < m_k < 1$ and $\gamma_0^{lsqr} = \|A\|$. For $k = 1, 2, \dots, n-2$, the strict monotonic decreasing property holds:

$$(6.14) \quad \|A^T A - Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T\| < \|A^T A - Q_{k+2} Q_{k+2}^T A^T A Q_{k+1} Q_{k+1}^T\|.$$

Proof. Combining (6.9) with (3.5) and (3.7), for $k = 2, 3, \dots, n-1$ we obtain from [48, p.98] and [7, p.218] that

$$(6.15) \quad \|F_k\|^2 = \|G_k\|^4 + m'_k \alpha_{k+1}^2 \beta_{k+1}^2 \leq (\gamma_k^{lsqr})^4 + m_k (\gamma_{k-1}^{lsqr} \gamma_k^{lsqr})^2$$

with $0 < m'_k \leq 1$ and $0 < m_k < m'_k$, from which the lower and upper bounds in (6.13) follow directly.

For $k = 1$, the equality in (6.15) is still true. From (3.7), we have $\alpha_2 < \gamma_1^{lsqr}$, $\beta_2 < \|A\| = \gamma_0^{lsqr}$. Therefore, we obtain

$$(\gamma_1^{lsqr})^4 < \|F_1\|^2 = \|G_1\|^4 + m'_1 \alpha_2^2 \beta_2^2 \leq (\gamma_1^{lsqr})^4 + m_1 (\gamma_0^{lsqr} \gamma_1^{lsqr})^2,$$

from which it follows that (6.13) holds for $k = 1$.

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 " $<$ ". Since $B_n^T B_n = Q_n^T A^T A Q_n$ is an unreduced symmetric tridiagonal matrix, its singular values σ_i^2 , $i = 1, 2, \dots, n$ are simple. Observe that F_k is the matrix deleting the first k columns of $B_n^T B_n$ and the first k zero rows of the resulting matrix. Consequently, the singular values $\zeta_i^{(k)}$, $i = 1, 2, \dots, n-k$ of F_k strictly interlace the simple singular values σ_i^2 , $i = 1, 2, \dots, n$ of $B_n^T B_n$ and are thus simple for $k = 1, 2, \dots, n-1$. Moreover, the singular

values of F_{k+1} strictly interlace those of F_k , which means that $\zeta_1^{(k)} < \zeta_1^{(k+1)}$, i.e., $\|F_k\| < \|F_{k+1}\|$, which proves (6.14). \square

REMARK 6.1. According to the results and analysis in [33], we have $\gamma_{k-1}^{lsqr}/\gamma_k^{lsqr} \sim \rho$ for severely ill-posed problems, and $\gamma_{k-1}^{lsqr}/\gamma_k^{lsqr} \sim (k/(k-1))^\alpha$ for moderately and mildly ill-posed problems. Therefore, the lower and upper bounds of (6.13) indicate that $\|A^T A - Q_{k+1} Q_{k+1}^T A^T A Q_k Q_k^T\| \sim (\gamma_k^{lsqr})^2$.

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 6.3. Let $(\tilde{\theta}_1^{(k)})^2 > (\tilde{\theta}_2^{(k)})^2 > \dots > (\tilde{\theta}_k^{(k)})^2$ be the singular values of $(B_k^T B_k, \alpha_{k+1} \beta_{k+1} e_k^{(k)})^T$. Then for $i = 1, 2, \dots, k$ we have

$$(6.16) \quad \theta_i^{(k)} < \tilde{\theta}_i^{(k)} < \sigma_i,$$

$$(6.17) \quad (\tilde{\theta}_i^{(k)})^2 < (\theta_i^{(k)})^2 + \gamma_k^{lsqr} \gamma_{k-1}^{lsqr}.$$

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 σ_i , $i = 1, 2, \dots, n$, 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 σ_i^2 of $B_n^T B_n$:

$$\sigma_{n-k+i}^2 < (\tilde{\theta}_i^{(k)})^2 < \sigma_i^2, \quad i = 1, 2, \dots, k$$

and are simple, which means the upper bound (6.16).

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 (6.16).

On the other hand, we have

$$(B_k^T B_k, \alpha_{k+1} \beta_{k+1} e_k^{(k)}) (B_k^T B_k, \alpha_{k+1} \beta_{k+1} e_k^{(k)})^T = (B_k^T B_k)^2 + \alpha_{k+1}^2 \beta_{k+1}^2 e_k^{(k)} (e_k^{(k)})^T.$$

Recall (3.6) that $\alpha_{k+1} < \gamma_k^{lsqr}$ and $\beta_{k+1} < \gamma_{k-1}^{lsqr}$. By standard perturbation theory, we obtain

$$(\tilde{\theta}_i^{(k)})^4 - (\theta_i^{(k)})^4 \leq \alpha_{k+1}^2 \beta_{k+1}^2 < (\gamma_k^{lsqr} \gamma_{k-1}^{lsqr})^2, \quad i = 1, 2, \dots, k,$$

from which it follows that (6.17) holds. \square

REMARK 6.2. (6.16) indicates that $\tilde{\theta}_i^{(k)}$, $1 = 1, 2, \dots, k$ approximate the first k large singular values σ_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 $\theta_k^{(k)} < \sigma_{k_0+1}$. A combination of this and the previous analysis on the semi-convergence of CGME and LSQR implies that the semi-convergence of LSMR must occur no sooner than that of LSQR. On the other hand, (6.17) shows that $\tilde{\theta}_i^{(k)}$ is bounded from the above by $\theta_i^{(k)}$ as an approximation to σ_i , which and (6.16) imply that $\tilde{\theta}_i^{(k)}$ and $\theta_i^{(k)}$ interact and $\theta_i^{(k)}$ cannot be considerably more accurate than $\tilde{\theta}_i^{(k)}$ as approximations to the large singular values of A for $i = 1, 2, \dots, k$.

REMARK 6.3. A combination of Theorem 6.1 and the above two remarks means 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 results on LSQR in Section 3, we conclude that LSMR has the full regularization for severely or moderately ill-posed problems with suitable $\rho > 1$ or $\alpha > 1$.

A final note is that Huang and Jia [31] have derived the eigendecomposition, i.e., equivalent SVD, filtered expansion of MINRES iterates for $Ax = b$ with A symmetric; see Theorem 3.1 there. The result can be directly adapted to the LSMR iterates x_k^{lsmr} by keeping in mind that LSMR is mathematically equivalent to MINRES applied to the specific symmetric positive definite linear system $A^T Ax = A^T b$.

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, LSMR and MCGME on almost all the 1D and 2D problems from [2, 23, 25] 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). We mention that the relatively easy 1D problems are all from [23, 25], where *shaw*, *gravity* and *baart* are severely ill-posed and *phillips*, *heat* and *deriv2* are moderately. The 2D image deblurring problems *blur*, *fanbeamtomo* and *seismictomo* are also from [23, 25], and the other 2D problems are from [2]. We notice that for *blur*, *fanbeamtomo*, although the orders m and n are already tens of thousands, their condition numbers σ_1/σ_n are only 31.5 and 2472, respectively, which, intuitively, do not satisfy the definition of a discrete ill-posed problem whose singular values decay and are centered at zero, so that the ratio σ_1/σ_n is very large. For each test problem, we compute $b_{\text{true}} = Ax_{\text{true}}$ and add a Gaussian white noise e with zero mean to b_{true} by prescribing the relative noise level

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

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

For all the 1D problems and the 2D *seismictomo*, we report the results on them for $\varepsilon = 10^{-3}$; for all the 2D problems except *blur* and *fanbeamtomo*, we report the results on them for $\varepsilon = 5 \times 10^{-3}$. For several other $\varepsilon \in [10^{-3}, 5 \times 10^{-2}]$, we have the same findings. For *blur* and *fanbeamtomo*, however, we will observe some fundamental distinctions between the convergence features for ε lying in this practical interval. Figures 2–7 depict the convergence processes of LSQR, CGME, LSMR and MCGME, and we give some key details, including the iterations k^* at which the semi-convergence of an algorithm occurs and the relative error of the best regularized solution obtained by each algorithm, which is defined by

$$\frac{\|x_{k^*}^{lsqr} - x_{\text{true}}\|}{\|x_{\text{true}}\|}$$

for LSQR. Similar relative errors are defined for CGME, LSMR and MCGME with the superscript “*lsqr*” replaced by “*cgme*”, “*lsmr*” and “*mcgme*”, respectively. In addition, as a comparison standard on the solution accuracy, we depict the semi-convergence process of the TSVD method for *blur* and *seismictomo*, and report the

TABLE 1
The description of test problems.

Problem	Description	Size of m, n
shaw	1D image restoration model	$m = n = 5000$
gravity	1D gravity surveying problem	$m = n = 5000$
baart	1D image deblurring	$m = n = 5000$
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 Turbulence Blur	$m = n = 65536$
GaussianBlur422	Spatially Invariant Atmospheric Turbulence Blur	$m = n = 65536$
VariantGaussianBlur1	Spatially Variant Gaussian Blur	$m = n = 99856$
VariantGaussianBlur2	Spatially Variant Gaussian Blur	$m = n = 99856$
VariantMotionBlur_large	Spatially Variant Motion Blur	$m = n = 65536$
VariantMotionBlur_medium	Spatially Variant Motion Blur	$m = n = 65536$
blur	2D image restoration	$m = n = 22500$
fanbeamtomo	2D fan-beam tomography problem	61200×14400
seismictomo	2D seismic tomography	20000×10000

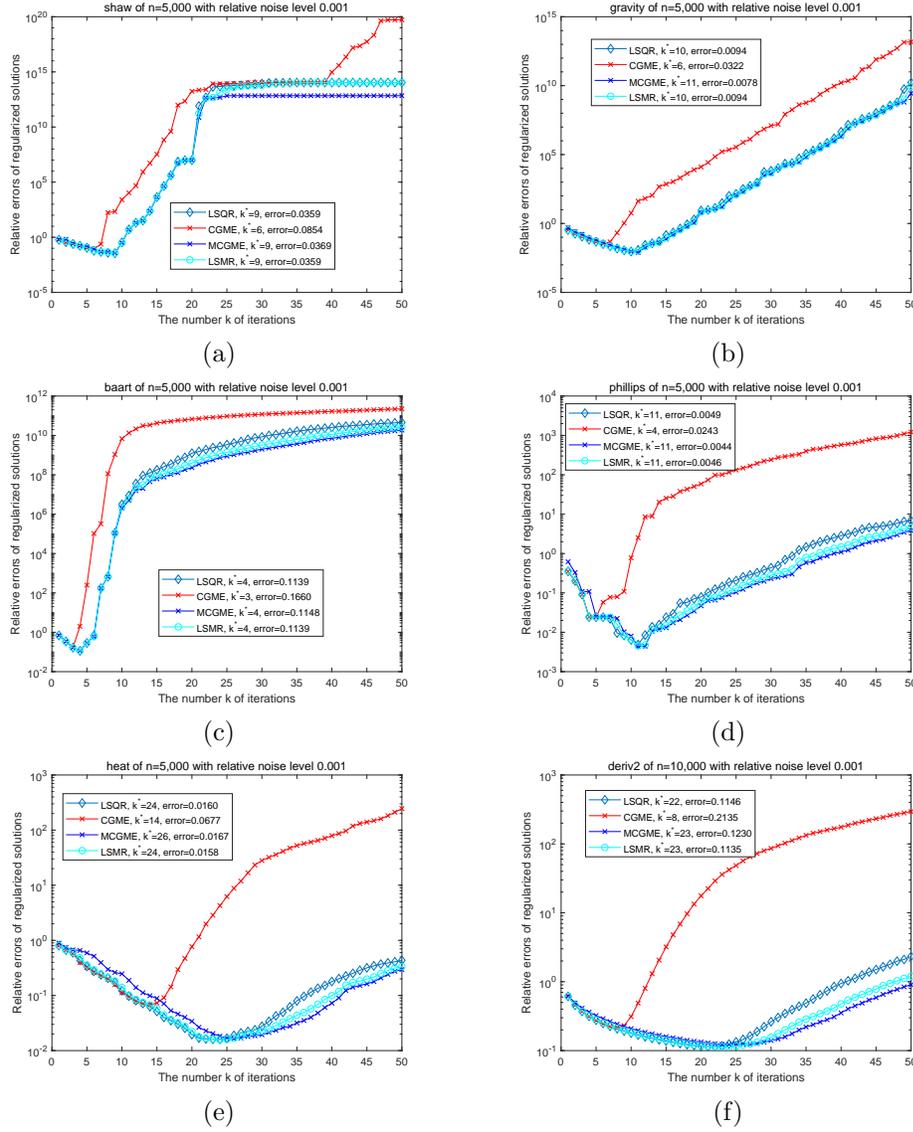
relative errors of the best TSVD regularized solutions $x_{k_0}^{tsvd}$ with k_0 the transition point at which the semi-convergence of TSVD occurs. For the other nine larger 2D problems, we cannot compute the SVDs of the matrices due to out of memory in our computer. We mention that for the first six 1D test problems we have found that the best regularized solutions obtained by TSVD method have the same accuracy as those by LSQR, where the k_0 are very small relative to n and all the $k^* \leq k_0$ correspondingly. We omit the results on the 1D problems obtained by the TSVD method.

We now comment the figures and the related details in order.

Firstly, for all the problems in Table 1, the semi-convergence of CGME occurs earlier than LSQR and can be much earlier. This confirms Theorem 4.4. The much earlier semi-convergence of CGME indicates that $\tilde{\theta}_k^{(k)} < \sigma_{k_0+1}$ occurs much earlier for CGME than $\theta_k^{(k)} < \sigma_{k_0+1}$ for LSQR.

Secondly, for all the problems, the best regularized solutions $x_{k^*}^{cgme}$ are correspondingly less accurate than $x_{k^*}^{lsqr}$ considerably except for blur in Figure 5, where the best regularized solution by CGME is almost as accurate as those by LSQR, LSMR and MCGME. For all the 1D problems but baart 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 the other three ones, indicating that the regularization ability is considerably inferior to the other three ones, given that the relative errors by LSQR, LSMR and MCGME themselves are only roughly $0.01 \sim 0.1$; see Figures 1 (a) and 6 (a). These results confirm Theorems 4.1–4.2 and the analysis on them. We will make more comments on Figure 5 later.

Thirdly, for each of the problems, by a careful observation and comparison, we have found that x_k^{cgme} is more accurate than and at least at least as accurate as x_k^{lsqr}

FIG. 1. 1D problems with the relative noise level $\varepsilon = 10^{-3}$.

until the occurrence of CGME, after which LSQR continues improving iterates until the occurrence of its semi-convergence, as is clearly seen from Figures 1–7. 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 only slightly smaller than that of $x_{k^*}^{lsqr}$, and there is little difference between them. 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 6.2 and justify that LSMR has the

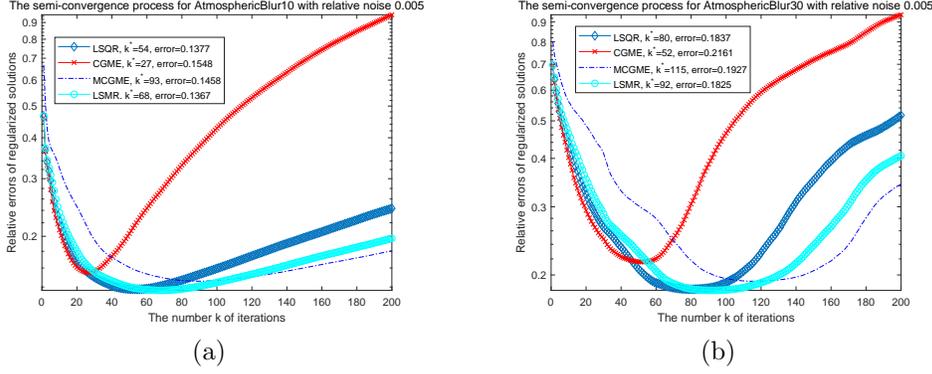


FIG. 2. (a): AtmosphericBlur10 and (b): AtmosphericBlur30 with $\varepsilon = 5 \times 10^{-3}$.

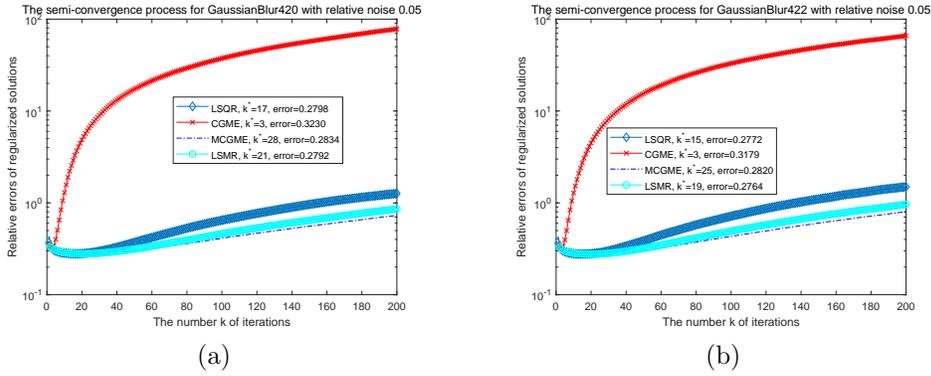


FIG. 3. (a): GaussianBlur420 and (b): GaussianBlur422 with $\varepsilon = 5 \times 10^{-3}$

same regularization ability as that of LSQR.

Fifthly, for each of the test problems, MCGME improves CGME substantially. As a matter of fact, for the 1D problems, the best regularized solutions by MCGME have the same accuracy as those by LSQR and LSMR; for the 2D problems, the best regularized solutions $x_{k^*}^{mcmge}$ are almost as accurate as $x_{k^*}^{lsqr}$ and $x_{k^*}^{lsmr}$.

Sixthly, as we have stated, *blur* and *fanbeamtomo* are quite well conditioned. With the relatively small $\varepsilon = 10^{-3}$, we observe from Figures 5–6 that there is no semi-convergence phenomenon for LSQR, LSMR and MCGME as well as the TSVD method. This means that e does not play a part in regularization and these methods solve these two problems as if they were ordinary linear systems. Furthermore, it is clear from the figures that the relative errors of regularized solutions obtained by LSQR, LSMR and MCGME stabilize after 30 iterations for *blur* and 80 iterations for *fanbeamtomo*, respectively. Figures 5 (a) and 6 (a) seems to indicate that CGME has no semi-convergence phenomenon for the *square blur* and given ε but it has for the *rectangular fanbeamtomo*. However, this semi-convergence is in disguise and is not caused by the noise e : For the rectangular *fanbeamtomo*, (4.15), its proof and the analysis on it state that the smallest singular value $\bar{\theta}_k^{(k)}$ of \bar{B}_k can be arbitrarily small and approaches zero as k increases. As we have elaborated, $(\bar{\theta}_k^{(k)})^2$ approaches the eigenvalue zero of AA^T as k increases. As a result, the projected problem $\bar{B}_k y_k^{cgme} =$

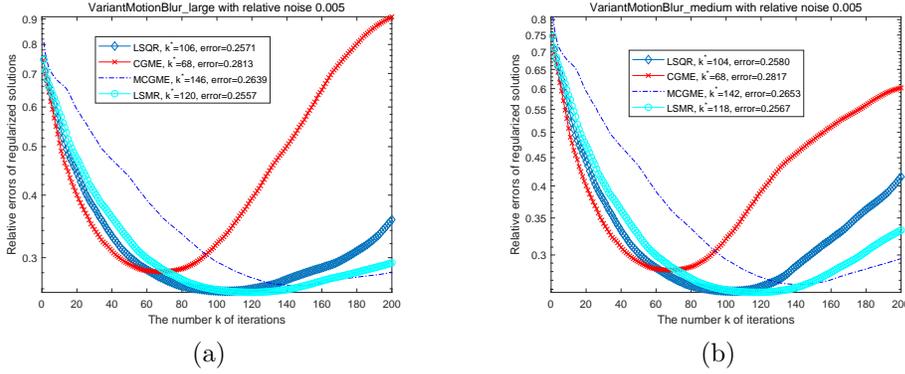


FIG. 4. (a): VariantMotionBlur_large and (b): VariantMotionBlur_medium with $\varepsilon = 5 \times 10^{-3}$.

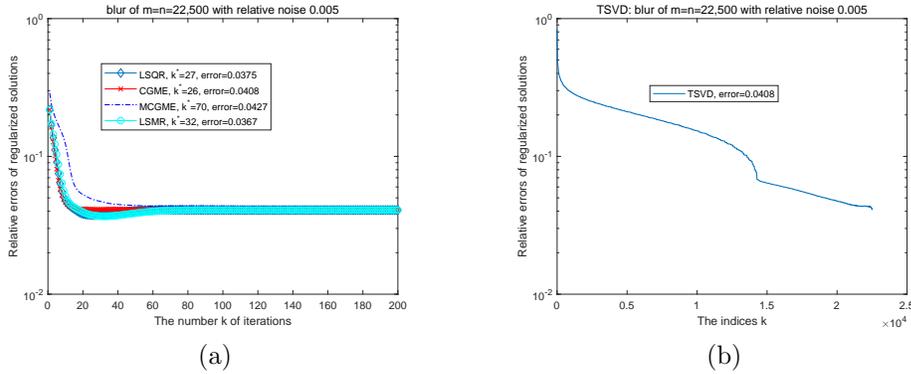
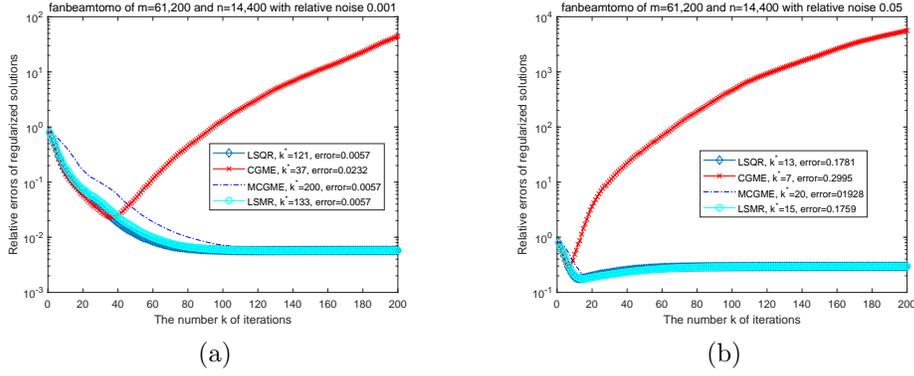
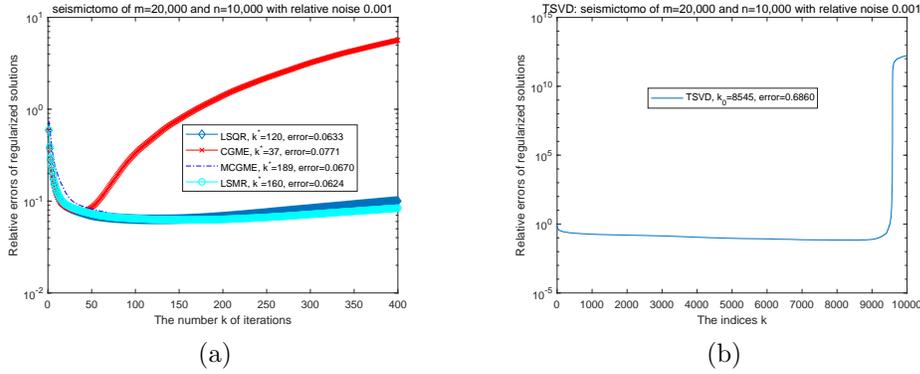


FIG. 5. blur.

$\beta e_1^{(k)}$ involved in CGME can become even worse conditioned than (1.1) itself as k increases for A rectangular, causing that $\|x_k^{cgme}\|$, which equals $\|Q_k y_k^{cgme}\| = \|y_k^{cgme}\|$, and the relative error $\frac{\|x_k^{cgme} - x_{true}\|}{\|x_{true}\|}$ tends to infinity with respect to k . This can also be seen from (4.20), where we can easily check that $|f_k^{(k,cgme)}| \rightarrow \infty$ as k increases since σ_k is a constant but $\bar{\theta}_k^{(k)} \rightarrow 0$ as k increases.

In contrast, the smallest singular values of the projection matrices are always bounded from below by either σ_n for LSQR (cf. (4.14)) and MCGME (cf. (4.30)) or σ_n^2 for LSMR (cf. (6.16)), no matter how A is rectangular or square. This is why CGME has seemingly semi-convergence phenomenon for A rectangular when the other solvers do not have. In the meantime, we see that the best regularized solution by CGME is substantially less accurate than those by the other three algorithms for *fanbeamtomo*. For the square *blur* with $\varepsilon = 10^{-3}$, we see that the four Krylov solvers and the TSVD method do not exhibit semi-convergence and compute the solutions with very comparable accuracy. These results and analysis tell us that CGME is definitely not a good choice when A is rectangular.

Seventhly, if the relative noise level ε is increased to $\varepsilon = 0.05$, the semi-convergence of LSQR, LSMR and MCGME occurs for *fanbeamtomo*, as is seen from Figure 6. We have also observed the semi-convergence of the four algorithms and the TSVD method for *blur* with $\varepsilon = 0.05$. We find that the best regularized solutions by LSQR, LSMR

FIG. 6. fanbeamtomography with $\varepsilon = 10^{-3}$ and 5×10^{-2} .FIG. 7. seismic tomography with $\varepsilon = 10^{-3}$.

and MCGME have very comparable accuracy but CGME computes a less accurate best regularized solution. We omit the corresponding figure. For the test problems, we have also observed that the semi-convergence of the TSVD method occurs much later than the four Krylov solvers, i.e., $k^* \ll k_0$.

8. Conclusions. For a general large-scale ill-posed problem (1.1), iterative solvers are only computationally viable. Of them, the Krylov solvers LSQR, CGLS, CGME and LSMR have been commonly used. In terms of the accuracy of the rank k approximation to A in LSQR, in this paper we have derived accurate estimates for the accuracy of the rank k approximations to A and $A^T A$ that are involved in CGME and LSMR, respectively. We have made detailed analyses on the approximation behavior of the singular values of the projection matrices associated with CGME and LSMR. In the meantime, we have derived the filtered SVD expansion of CGME regularized iterates. In conclusion, we have shown that the regularization of CGME is generally inferior to LSQR and the semi-convergence of CGME occurs no later than that of LSQR. We have extracted a best possible rank k approximation to A from the rank $(k+1)$ approximation $P_{k+1} P_{k+1}^T A$, and have shown why such approximation is as accurate as the rank k approximation in LSQR. Based on this analysis, as a by-product, we have proposed a modified CGME (MCGME) method that improves CGME substantially and has the same regularization ability as LSQR.

We have substantially 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 unconditionally superior to theirs and reveal how the truncation step affects the accuracy of the truncated rank k approximation to A .

In the meantime, we have proved that LSMR has the same regularization ability 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 confirm our regularization results on CGME and LSMR. We have also numerically demonstrated that the best regularized solutions by MCGME are very comparable to those by LSQR.

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