Regularization properties of LSQR for linear discrete ill-posed problems in the multiple singular value case and best, near best and general low rank approximations

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Abstract

For the large-scale linear discrete ill-posed problem \( \min \| Ax - b \| \) or \( Ax = b \) with \( b \) contaminated by white noise, the Golub–Kahan bidiagonalization based LSQR method and its mathematically equivalent CGLS, the conjugate gradient (CG) method applied to \( A^T A x = A^T b \), are most commonly used. They have intrinsic regularizing effects, where the iteration number \( k \) plays the role of regularization parameter. The long-standing fundamental question is: Can LSQR and CGLS find two-norm filtering best possible regularized solutions? The author has given definitive answers to this question for severely and moderately ill-posed problems when the singular values of \( A \) are simple. This paper extends the results to the multiple singular value case, and studies the approximation accuracy of Krylov subspaces, the quality of low rank approximations generated by Golub–Kahan bidiagonalization and the convergence properties of Ritz values. For the two kinds of problems, we prove that LSQR finds two-norm filtering best possible regularized solutions at semi-convergence. Particularly, we consider some important and untouched issues on best, near best and general rank \( k \) approximations to \( A \) for the ill-posed problems with the singular values \( \sigma_k = O(k^{-\alpha}) \) with \( \alpha > 0 \), and the relationships between them and their nonzero singular values. Numerical experiments confirm our theory. The results on general rank \( k \) approximations and the properties of their nonzero singular values apply to several Krylov solvers, including LSQR, CGME, MINRES, MR-II, GMRES and RRGMRES.

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(Some figures may appear in colour only in the online journal)

1. Introduction and preliminaries

Consider the linear discrete ill-posed problem

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

where the norm $\| \cdot \|$ is the two-norm of a vector or matrix, and $A$ is extremely ill conditioned with its singular values decaying to zero without a noticeable gap. Without loss of generality, we assume that $m \geq n$. Problem (1) typically arises from the discretization of Fredholm integral equation of the first kind:

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

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. If $k(s, t)$ is non-degenerate and $g(s)$ satisfies the Picard condition, there exists the unique square integrable solution $x(t)$; see [12, 23, 25, 40, 41]. Here for brevity we assume that $s$ and $t$ belong to the same set $\Omega \subset \mathbb{R}^q$ with $q \geq 1$. Applications include image deblurring, signal processing, geophysics, computerized tomography, heat propagation, biomedical and optical imaging, groundwater modeling, and many others; see, e.g., [1, 11, 12, 25, 37, 40–42, 53]. 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) bears no relation to the true solution $x_{true} = A^\dagger b_{true}$, where $\dagger$ 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 $e$, we always assume that $b_{true}$ satisfies the discrete Picard condition $\|A^\dagger b_{true}\| \leq C$ with some constant $C$ for $n$ arbitrarily large [1, 22, 23, 25, 38]. It is an analog of the Picard condition in the finite dimensional case; see, e.g., [23, p 9], [25, p 12] and [38, p 63]. Without loss of generality, assume that $Ax_{true} = b_{true}$. Then one can solve one of the following mathematically equivalent regularization problems:

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

with $\tau \approx 1$ and general-form Tikhonov regularization

$$\min_{x \in \mathbb{R}^n} \{\|Ax - b\|^2 + \lambda^2 \|Lx\|^2\}$$

with $\lambda > 0$ the regularization parameter [23, 25], where $L$ is a regularization matrix and its suitable choice is based on a-priori information on $x_{true}$. Typically, $L$ is either the identity matrix $I$ or the scaled discrete approximation of a first or second order derivative operator. If $L = I$, (4) is standard-form Tikhonov regularization, and both (3) and (4) are two-norm filtering regularization problems. If $L \neq I$, problems (3) and (4), in principle, can be transformed into standard-form problems [23, 25]. However, transformation to standard form is practically feasible only when $L$ is easily invertible or a linear system or least squares problem with $L$ can be easily solved.
We are concerned with the case $L = I$ in this paper. When $L = I$, for problem (3) of small or moderate size, an effective and reliable solution method is the truncated singular value decomposition (TSVD) method, and it obtains the two-norm filtering best regularized solution $x_{\text{tsvd}}^k$ at some $k_0 < n$ [23, 25], where $k_0$ is the optimal regularization parameter, called the transition point, such that $\|x_{\text{tsvd}}^k - x_{\text{true}}\| = \min_{k=1,2,\ldots}\|x_{\text{tsvd}}^k - x_{\text{true}}\|$. We will review the TSVD method and reformulate it and (4) when $A$ has multiple singular values. A key of solving (4) is the determination of the optimal regularization parameter $\lambda_{\text{opt}}$, such that $\|x_{\lambda_{\text{opt}}} - x_{\text{true}}\| = \min_{\lambda > 0}\|x_{\lambda} - x_{\text{true}}\|$. A number of parameter-choice methods have been developed for finding $\lambda_{\text{opt}}$, such as the discrepancy principle, the L-curve criterion, and the generalized cross validation (GCV), etc. We refer the reader to, e.g., [23, 25] for details.

It has been theoretically and numerically justified that $x_{\lambda_{\text{opt}}}$ essentially have the minimum two-norm error; see [22, 52], [23, pp 109–111] and [25, sections 4.2 and 4.4]. In effect, the theory in [12] has shown that the error of $x_{\lambda_{\text{opt}}}$ is unconditionally order optimal in the finite dimensional space setting, i.e., the same order as the worst case error [12, sections 3.3 and p 78], where $x_{\lambda_{\text{opt}}}$ is order optimal only when the worst case error is no less than $O(\|e\|^2)$ for $\|e\|$ sufficiently small and thus conditionally optimal; see [12, pp 119–120] and [40, theorems 2.12–2.13, pp 38–39] for details. As a result, we can naturally take $x_{\lambda_{\text{opt}}}$ as a reference standard when assessing the regularization ability of a two-norm filtering regularization method.

For problem (1) large, the TSVD method and the Tikhonov regularization method are generally too demanding, and only iterative regularization methods are computationally viable. Krylov iterative solvers are a major class of methods for solving (1), and they project problem (1) onto a sequence of low dimensional Krylov subspaces and computes iterates to approximate $x_{\text{true}}$ [1, 12, 17, 18, 23, 25, 40]. Of them, the CGLS method, which implicitly applies the CG method [26] to $\mathbf{A}^T\mathbf{A}x = \mathbf{A}^Tb$, and its mathematically equivalent LSQR algorithm [45] have been most commonly used. The Krylov solvers CGME [4, 5, 10, 18, 19] and LSMR [5, 14] are also choices. These Krylov solvers have general regularizing effects [1, 17–19, 23, 25, 27, 28] and exhibit semi-convergence [42, p 89]; see also [4, p 314], [23, p 135] and [25, p 110]: the iterates converge to $x_{\text{true}}$ in an initial stage; afterwards the noise $e$ starts to deteriorate the iterates so that they start to diverge from $x_{\text{true}}$ and instead converge to $x_{\text{naive}}$. If we stop at the right time, then, in principle, we have a regularization method, where the iteration number plays the role of the regularization parameter. Semi-convergence is due to the fact that the projected problem starts to inherit the ill-conditioning of (1) from some iteration onwards, and the appearance of a small singular value of the projected problem amplifies the noise considerably.

The behavior of (1), (3) and (4) with $L = I$ critically depends on the decay rate of the singular values $\sigma_j$ of $A$. For a linear compact operator equation such as (2) in the Hilbert space setting, let $\mu_1 \geq \mu_2 \geq \cdots \geq 0$ be the singular values of the compact operator $K$. The following characterization of the degree of ill-posedness of (2) was introduced in [29] and has been widely used; see, e.g. [1, 12, 23, 25, 41]: if $\mu_j = O(\rho^{-j})$ with $\rho > 1, j = 1, 2, \ldots, \infty$, then (2) is severely ill-posed; if $\mu_j = O(\rho^{-j\alpha})$, then (2) is mildly or moderately ill-posed for $\frac{1}{\alpha} < \alpha \leq 1$ or $\alpha > 1$. Here for mildly ill-posed problems we add the requirement $\alpha > \frac{1}{2}$, which does not appear in [29] but must be met for a linear compact operator equation [20, 23]. In the one dimensional case, i.e., $q = 1$, (1) is severely ill-posed when the kernel function $k(s, t)$ is sufficiently smooth, and it is moderately ill-posed with $\mu_j = O(j^{-p-1/2})$, where $p$ is the highest order of continuous derivatives of $k(s, t)$; see, e.g., [23, p 8] and [25, pp 10–11]. The singular values $\sigma_j$ of discretized problem (1) resulting from the continuous (2) inherit the decay properties of $\mu_j$ [23, 25], provided that discretizations are fine enough, so that the classification applies to problem (1) as well.
Björck and Eldén in their 1979 survey [6] foresightedly expressed a fundamental concern on CGLS (and LSQR): more research is needed to tell for which problems this approach will work, and what stopping criterion to choose. See also [23, p 145], Hanke and Hansen [20] and Hansen [24] address that a strict proof of the regularizing properties of conjugate gradients (CG) is extremely difficult. Over the years, an enormous effort has been made to the study of regularizing effects of LSQR and CGLS; see, e.g. [13, 19, 23, 25, 27, 28, 30, 33, 34, 40, 43, 46, 48]. To echo the concern of Björck and Eldén, such a definition has been introduced in [30, 33]: if a regularized solution to (1) is at least as accurate as $x_{\text{svd}}$, then it is called a best possible two-norm filtering regularized solution. If the regularized solution by an iterative regularization solver at semi-convergence is such a best possible one, then the solver is said to have the full regularization. Otherwise, the solver is said to have only the partial regularization.

Since it had been unknown whether or not LSQR, CGME and LSMR have the full regularization for a given (1), one commonly combines them with some explicit regularization [1, 23, 25]. The hybrid LSQR variants have been advocated by Björck and Eldén [6] and O’Leary and Simmons [44], and improved and developed by Björck [3], Björck, Grimme and van Dooren [7], and Renault et al [47]. A hybrid LSQR first projects (1) onto Krylov subspaces and then regularizes the projected problems explicitly. It aims to remove the effects of small Ritz values and expands Krylov subspaces until they captures all needed dominant SVD components of $A$ [3, 7, 20, 44], so that the error norms of regularized solutions and the residual norms possibly decrease further until they ultimately stabilize. The hybrid LSQR, CGME and LSMR have been intensively studied in, e.g., [2, 8, 9, 19, 20, 47] and [1, 25]. However, as opposed to one’s common expectations, there may be some intrinsic mathematical difficulties, which may critically affect the solution accuracy and a reliable design of stopping criteria of hybrid algorithms; see [36] for elaborations and experiments.

If an iterative solver itself, e.g., LSQR, is theoretically proved and practically identified to have the full regularization, one simply stops it after a few iterations of semi-convergence, and no complicated hybrid variant is needed. In computation, some parameter-choice methods, such as the L-curve criterion, the discrepancy principle and generalized cross validation (GCV) method, can be used to estimate the point of semi-convergence so as to stop iterations properly. Therefore, we cannot emphasize too much the importance of proving the full or partial regularization of LSQR, CGLS, CGME and LSMR. By the definition of the full or partial regularization, a fundamental question is: Do LSQR, CGLS, LSMR and CGME have the full or partial regularization for severely, moderately and mildly ill-posed problems?

Regarding LSQR and CGLS, for the three kinds of ill-posed problems described above, the author [33, 34] has proved that LSQR has the full regularization for severely and moderately ill-posed problems with certain suitable $\rho > 1$ and $\alpha > 1$ under the assumption that all the singular values of $A$ are simple. In [35], the author has given a detailed analysis on CGME and LSMR and established close relationships between them and LSQR, showing that LSMR has the same regularization ability as LSQR and the regularizing effects of CGME are generally inferior to those of LSQR.

There are numerous important applications where the matrices $A$’s have multiple singular values. Typical applications include 2D image deblurring or restoration problems, tomographic reconstruction problems and inverse diffusion problems, which arise in astronomy, microscopy and crowd surveillance, etc [15]. As a matter of fact, we have found that four of the twelve 2D test problems collected in [15] in a variety of applications belong to the multiple singular value case. They are the severely ill-posed image deblurring problem PRblurgauss, the mildly ill-posed image deblurring problem PRblurrotation, the mildly ill-posed computerized tomography problem PRtomo, and the severely ill-posed nuclear magnetic resonance (NMR) relaxometry problem PRnmr. In the continuous setting, a mathematical model of
image deblurring problems can be expressed as the integral form (2), where the kernel \(k(s, t)\) is a function that specifies how the points in the image are distorted and is called the point spread function (PSF). Typical problems are spatially invariant and variant Gaussian blurs, where the kernels \(k(s, t)\)'s are Gaussian PSFs that are both symmetric and separable with some practical parameters [2], i.e., \(k(s, t) = k_1(s)k_1(t)\). Other afore-mentioned 2D ill-posed problems can also be written as the form (2) with different integral domains \(\Omega\). Whenever the kernel \(k(s, t)\) in (2) is symmetric and separable and the same discretization scheme is applied to \(k_1(s)\) and \(k_1(t)\) with respect to \(s \in \Omega\) and \(t \in \Omega\), respectively, the resulting matrix \(A\) has the Kronecker product form \(A = C \otimes C\) with \(C\) a square matrix and thus its singular values must be multiple.

In this paper, we extend the regularization results on LSQR in [33, 34] to the multiple singular value case. In section 2, we reformulate the TSVD method and standard-form Tikhonov regularization in the multiple singular value case, showing that they compute regularized solutions as if they work on a modified form of (1), where the coefficient matrix \(A'\) has the \(s\) distinct singular values of \(A\) as its nonzero simple singular values and the other singular values are zero with the multiplicity \(n - s\). In section 3, we show that LSQR works as if it solves the same modified one of (1). In this way, we build a bridge that connects the regularizing effects of the TSVD method and those of LSQR, so that we can analyze the regularization ability of LSQR by taking the best TSVD regularized solution as the reference standard. In sections 4–6, we extend some of the main results in [33, 34] to the multiple singular value case, whose proofs need some nontrivial changes in the original ones of [33, 34]; we state some important results in [33, 34] that not only need numerical justifications in the multiple singular value case but also are indispensable in the topics to be described in the next paragraph, though their proofs are straightforward from the corresponding proofs in [33, 34]. On the other hand, we omit those results which do not play an essential role in this paper and whose proofs are from [33, 34] without any change. Finally, we draw the same conclusions as those in [33, 34].

After the above, we consider some important issues that have received no attention in the literature: best, near best and general rank \(k\) approximations to \(A\) for the ill-posed problems with \(\alpha > 1\) and \(0 < \alpha \leq 1\), respectively, which include mildly ill-posed problems, and some intrinsic relationships between them and the approximation properties of their nonzero singular values. These results apply to LSQR, where the Ritz values, i.e., the nonzero singular values of rank \(k\) approximation matrices generated by Golub–Kahan bidiagonalization, critically decide the regularization ability of LSQR. As we will show, unlike for severely and moderately ill-posed problems with suitable \(\rho > 1\) and \(\alpha > 1\), a best or near best rank \(k\) approximation to \(A\) does not mean that its nonzero singular values approximate the large singular values of \(A\) in natural order, and such a rank \(k\) approximation matrix may have nonzero singular values that are (much) smaller than \(\sigma_{k+1}\). As a consequence, the importance and implication of this result is that replacing \(A\) by its excellent rank \(k\) approximation may be at risk in a variety of applications since such replacement may be unable to remove the effects of possible nonzero singular values (much) smaller than \(\sigma_{k+1}\). On this basis, we further consider the issue of general rank \(k\) approximations to \(A\) and analyze the rank \(k\) approximations to \(A\) involved in LSQR. Particularly, for \(0 < \alpha \leq 1\), given the accuracy of the rank \(k\) approximation in LSQR, we establish more insightful results on the nonzero singular values of the rank \(k\) approximation matrix, which estimate their maximum possible number that are smaller than \(\sigma_{k+1}\). These results also apply to the Krylov solvers CGME, MINRES and MR-II, and GMRES and RRGMRES [18, 25], each of which generates its own rank \(k\) approximation to \(A\) at iteration \(k\). All these constitute the work of section 7.

In section 8, we report the numerical experiments to confirm the results in sections 2 and 4–7. Finally, we conclude the paper in section 9.
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 $I$ and $0$ the identity matrix and the zero matrix whose orders are omitted whenever clear from the context.

2. The reformulation and analysis of the TSVD method and standard-form Tikhonov regularization in the multiple singular value case

In order to extend the results in [33, 34] to the multiple singular value case, we need to reorganize the SVD of $A$ and reformulate the TSVD method and standard-form Tikhonov regularization by taking $b$ in (1) into account carefully. To this end, we must make numerous necessary changes and preparations, as will be detailed below.

Let the SVD of $A$ be

$$A = \hat{U} \begin{pmatrix} \Sigma & 0 \\ 0 & 0 \end{pmatrix} \hat{V}^T,$$  

where $\hat{U} = (\hat{U}_1, \hat{U}_2, \ldots, \hat{U}_s) \in \mathbb{R}^{m \times m}$ with $\hat{U}_i \in \mathbb{R}^{m \times g_i}$ and $\hat{V} = (\hat{V}_1, \hat{V}_2, \ldots, \hat{V}_s) \in \mathbb{R}^{n \times g_s}$ with $\hat{V}_i \in \mathbb{R}^{n \times g_i}$ are orthogonal, $\Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_s, 0)$ with the $s$ distinct singular values $\sigma_1 > \sigma_2 > \cdots > \sigma_s > 0$, each $\sigma_i$ is $c_i$ multiple and $I_{c_i}$ the $c_i \times c_i$ identity matrix, and the superscript $T$ denotes the transpose of a matrix or vector. Then for a given Gaussian white noise $e$, by (5) we obtain

$$x_{\text{naive}} = \sum_{i=1}^{s} \frac{\hat{V}_i \hat{U}_i^T b}{\sigma_i} + \sum_{i=1}^{s} \frac{\hat{V}_i \hat{U}_i^T e}{\sigma_i} = x_{\text{true}} + \sum_{i=1}^{s} \frac{\hat{V}_i \hat{U}_i^T e}{\sigma_i},$$  

where $x_{\text{true}} = A^1 b_{\text{true}}$ with $\|x_{\text{true}}\| = \|A^1 b_{\text{true}}\| = \left(\sum_{i=1}^{s} \frac{\|\hat{U}_i^T b_{\text{true}}\|^2}{\sigma_i^2}\right)^{1/2}$, and the norm of the second term is very large (huge) for $\|e\|$ fixed.

The discrete Picard condition on (1) stems from the necessary requirement

$$\|x_{\text{true}}\| = \|A^1 b_{\text{true}}\| = \left(\sum_{i=1}^{s} \frac{\|\hat{U}_i^T b_{\text{true}}\|^2}{\sigma_i^2}\right)^{1/2} \leq C$$  

with some constant $C$, independent of $n$ and plays a fundamental role in the solution of linear discrete ill-posed problems; see, e.g. [1, 16, 22, 23, 25, 38, 47]. It states that, on average, the (generalized) Fourier coefficients $\|\hat{U}_i^T b_{\text{true}}\|$ decay faster than $\sigma_i$, which enables regularization to compute useful approximations to $x_{\text{true}}$. The following common model has been used throughout Hansen’s books [23, 25] and the references therein as well as [33, 34] and the current paper:

$$\|\hat{U}_i^T b_{\text{true}}\| = \sigma_i^{1+\beta}, \quad \beta > 0, \quad i = 1, 2, \ldots, s,$$  

where $\beta$ is a model parameter that controls the decay rates of $\|\hat{U}_i^T b_{\text{true}}\|$. We remark that Hansen [23, 25] uses the individual columns of $U_i$ in (7) if $\sigma_i$ is multiple, which is equivalent to assuming that each column of $U_i$ and the corresponding one of $\hat{V}_i$ makes the same contributions to $x_{\text{naive}}$ and $x_{\text{true}}$ and the TSVD method must use all the columns of $U_i$ and $\hat{V}_i$ associated with $\sigma_i$ to form a regularized solution. It is trivial to unify the discrete Picard condition on the individual columns of $U_i$ in the form of (7) for a multiple $\sigma_i$. 


Based on the above, in the multiple singular value case, the TSVD method [23, 25] solves (3) by dealing with the problem

$$\min \|x\| \ \text{subject to} \ \|A_k x - b\| = \min$$

for some $k$, where $A_k$ is a best rank $c_1 + c_2 + \cdots + c_k$ approximation to $A$ and the most common choice (see [4, p 12]) is

$$A_k = (\widehat{U}_1, \widehat{U}_2, \ldots, \widehat{U}_k)\Sigma_k(\widehat{V}_1, \widehat{V}_2, \ldots, \widehat{V}_k)^T$$

with $\Sigma_k = \text{diag}(\sigma_1 I_{c_1}, \sigma_2 I_{c_2}, \ldots, \sigma_k I_{c_k})$ and $\|A - A_k\| = \sigma_{k+1}$. The solution to (8) is $x_k^{\text{tvd}} = A_k^\dagger \tilde{b}$, where the index $k$ corresponds to the regularization parameter $c_1 + c_2 + \cdots + c_k$. Here it is worthwhile to point out that one might use some other matrix approximations of different ranks than $c_1 + c_2 + \cdots + c_k$, but this does not help and instead may cause some unnecessary troubles. For example, suppose that $c_k > 1$ and we use a best matrix approximation $A_k$ of rank bigger than $c_1 + c_2 + \cdots + c_k - 1$ but smaller than or equal to $c_1 + c_2 + \cdots + c_k$, i.e., the rank is $c_1 + c_2 + \cdots + c_k - 1 + c_k$ with $1 \leq c_k \leq c_k$. Then $A_k$ of form (9) is not unique for $k < c_k$ and, in fact, has infinitely many since $U_k$ and $V_k$ are now replaced by the matrices consisting of any $c_k$ left and right singular vectors of $A$ corresponding to $\sigma_k$, respectively. In this case, different $A_k$’s for $c_k = 1, 2, \ldots, c_k$ have the same approximation accuracy $\|A - A_k\| = \sigma_k$ for $c_k = c_k$ but $\|A - A_k\| = \sigma_{k+1}$ for $c_k = c_k$. However, the corresponding solutions to (8) with $A_k$ are different, and the errors of regularized solutions may decrease very slowly when $c_k$ varies from one to $c_k$. This can be easily understood since the regularized solution $A_k^\dagger \tilde{b}$ contains only the information on partial left and right singular subspaces of $A$ corresponding to $\sigma_k$ for $c_k < c_k$ but it may be essentially changed only after it contains the information on the full left and right singular subspaces of $A$ associated with $\sigma_k$. Our later numerical experiments will justify this assertion. In the meantime, for the purpose of this paper, the unique formulation (8) is absolutely necessary for our later reformulations of the TSVD method and Tikhonov regularization, which will form our starting point to consider the regularization of LSQR in the multiple singular value case.

In order to extend the results in [33, 34] to the multiple singular value case, the first key step is to take the right-hand side $b$ into consideration and to reorganize (5) so as to obtain an SVD of $A$ in some desired form by selecting a specific set of left and right singular vectors corresponding to a multiple singular value $\sigma_i$ of $A$. Specifically, for the $c_i$ multiple $\sigma_i$, $i = 1, 2, \ldots, s$, we choose an orthonormal basis of its left singular subspace by requiring that $b$ have a nonzero orthogonal projection on just one left singular vector $u_i$ in the singular subspace and no components in the remaining $c_1 - 1$ ones. Precisely, recall that the columns of $\widehat{U}_i$ form an orthonormal basis of the unique left singular subspace associated with $\sigma_i$. Then we must have

$$u_i = \frac{\widehat{U}_i \widehat{U}_i^T b}{\|\widehat{U}_i \widehat{U}_i^T b\|},$$

where $\widehat{U}_i \widehat{U}_i^T$ is the orthogonal projector onto the left singular subspace associated with $\sigma_i$. With such $u_i$, define the corresponding right singular vector $v_i = A_i^\dagger u_i / \sigma_i$, $i = 1, 2, \ldots, s$. We then select the other $c_1 - 1$ orthonormal left singular vectors which are orthogonal to $u_i$ and, together with $u_i$, form a new orthonormal basis of the left singular subspace associated with $\sigma_i$. We define the corresponding $c_1 - 1$ right singular vectors in the same way as $v_i$; they, together with $v_i$, form a new orthonormal basis of the right singular subspace associated with $\sigma_i$. 


Write the above resulting new left and right singular vector matrices as \( \tilde{U}_i \) and \( \tilde{V}_i \) with \( u_i \) and \( v_i \) as their first columns, respectively. Then \( \tilde{U}_i \) and \( \tilde{V}_i \) can be written as

\[
\tilde{U}_i = \tilde{U}_i Q_i, \quad \tilde{V}_i = \tilde{V}_i Q_i,
\]

where \( Q_i \) is a \( c_i \times c_i \) orthogonal matrix such that the first columns of \( \tilde{U}_i \) and \( \tilde{V}_i \) are \( u_i \) and \( v_i \), respectively. After such treatment, we obtain a desired compact SVD

\[
A = \tilde{U} \Sigma \tilde{V}^T
\]

with \( \tilde{U} = (\tilde{U}_1, \tilde{U}_2, \ldots, \tilde{U}_s) \) and \( \tilde{V} = (\tilde{V}_1, \tilde{V}_2, \ldots, \tilde{V}_s) \). We remind that \( u_i \) defined above is unique since the orthogonal projection of \( b \) onto the left singular subspace associated with \( \sigma_i \) is unique and does not depend on the choice of its orthonormal basis.

Although it is computationally unnecessary to construct \( \tilde{U}_i \) and \( \tilde{V}_i \) from given \( U_i \) and \( V_i \), \( i = 1, 2, \ldots, s \) in the current paper, we propose two efficient construction procedures, which may find potential applications in some other contexts. Computationally, given \( U_i \) and \( V_i \), \( i = 1, 2, \ldots, s \), once \( Q_i \) is available, we can construct \( \tilde{U}_i \) and \( \tilde{V}_i \) defined by (11) at cost of \( 2mc_i^2 \) flops and \( 2nc_i^2 \) flops, respectively. In what follows we show how to construct \( Q_i \) efficiently and stably by using either Householder transformation or the Gram–Schmidt orthogonalization procedure.

We now describe the first procedure. It follows from (11) that the construction is equivalent to finding an orthogonal matrix \( Q_i \). Since the first column of \( U_i \) is \( u_i \) defined by (10), the first column of \( Q_i \) is the \( c_i \)-dimensional unit-length vector \( \frac{v_i^T}{\|v_i^T\|} q \). Let \( P \) be the Householder transformation such that

\[
Pq = e_1
\]

with \( e_1 \) the first coordinate vector of dimension \( c_i \). Then the first column of \( P \) is \( q = Pe_1 \), and the second to the \( c_i \)th columns of \( P \) are mutually orthonormal and are orthogonal to \( q \). By exploiting the symmetry of \( P \), the explicit construction of \( P \) costs \( \frac{1}{2}c_i^2 \) flops approximately. By (10) we have

\[
\tilde{U}_i Pe_1 = \tilde{U}_i q = u_i.
\]

As a result, by the column orthonormality of \( \tilde{U}_i \), the second to the \( c_i \)th columns of \( \tilde{U}_i P \) are not only mutually orthonormal but also orthogonal to \( \tilde{U}_i Pe_1 = u_i \). This shows that \( P \) is a \( Q_i \) in (11). Consequently, we have obtained a desired \( \tilde{U}_i = \tilde{U}_i P \), whose explicit computation costs \( 2mc_i^2 \) flops approximately.

Alternatively, we can use the Gram–Schmidt orthogonalization procedure to construct a desired \( \tilde{U}_i \) in (11). To this end, we augment the above-defined \( q \) to a \( c_i \times c_i \) nonsingular matrix \( X = (q, \tilde{X}) \). We then perform the Gram–Schmidt orthogonalization procedure on \( X \) and compute the QR factorization \( X = QR \), which costs \( O((c_i - 1)^3) \) flops since the first column \( Qe_1 = q \) of the orthogonal matrix \( Q \) is known and need not be computed. Similarly, it can be straightforwardly justified that such \( Q \) is a \( Q_i \) satisfying (11) and produces a desired \( \tilde{U}_i \). The constant in the big \( O() \) ranges from 2 to 4 and depends on the reorthogonalization strategy for numerical stability in finite precision arithmetic, and with full reorthogonalization, the cost is \( 4(c_i - 1)^3 \) flops. Therefore, this procedure is more expensive than the Householder transformation approach when constructing a \( Q_i \). However, notice that \( c_i \) is generally very small and, for a given \( Q_i \), the cost of constructing \( \tilde{U}_i \) is \( 2mc_i^2 \) flops. Therefore, the cost of the Householder transformation procedure or the Gram–Schmidt orthogonalization procedure is negligible.
A few words for the construction of $X$ in practice: one can generate a $c_i \times (c_i - 1)$ matrix $\hat{X}$ randomly in a normal distribution. Such a way guarantees the non-singularity of $X$ in practice. Obviously, there are infinitely many $X$’s, each of which leads to its own $Q$, and delivers a different $\hat{U}_i$.

Now we need to prove that $\tilde{U}_i$ satisfies the discrete Picard condition (7). To see this, notice that

$$\|\tilde{U}_i^T b_{\text{true}}\| = \|Q_i^T \tilde{U}_i^T b_{\text{true}}\| = \|\tilde{U}_i^T b_{\text{true}}\| = \sigma_i^{1+\beta}, \quad i = 1, 2, \ldots, s.$$  \hfill (13)

Particularly, we have

$$|u_i^T b_{\text{true}}| \leq \|\tilde{U}_i^T b_{\text{true}}\| = \sigma_i^{1+\beta}, \quad i = 1, 2, \ldots, s.$$  \hfill (14)

We will take the equality when using (14) later, which does not affect all the proofs and results to be presented.

With (10) and (12), a crucial observation is that the solution $x_k^{\text{tsvd}}$ to (8) becomes

$$x_k^{\text{tsvd}} = A_i^T b = \sum_{i=1}^{k} \frac{u_i^T b}{\sigma_i},$$  \hfill (15)

which consists of the first $k$ large distinct dominant SVD components $(\sigma_i, u_i, v_i)$ of $A$.

Define the new $m \times n$ matrix

$$A' = US'V^T,$$  \hfill (16)

where $\Sigma' = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_s, 0) \in \mathbb{R}^{s \times n}$, $U = (u_1, u_2, \ldots, u_s, U_\perp) \in \mathbb{R}^{m \times n}$ and $V = (v_1, v_2, \ldots, v_s, V_\perp) \in \mathbb{R}^{n \times n}$ with $U_\perp$ and $V_\perp$ consisting of the other columns of $U$ and $V$ defined by (12), respectively.

Write

$$U = (U_i, U_\perp), \quad V = (V_i, V_\perp).$$  \hfill (17)

By construction, $A'$ has the $s$ nonzero simple singular values $\sigma_i, i = 1, 2, \ldots, s$ and $n - s$ multiple zero singular value, and $U_i^T b = 0$. We then see from (15) that the best rank $c_1 + c_2 + \cdots + c_k$ approximation $A_k$ to $A$ in (8) can be equivalently replaced by the best rank $k$ approximation

$$A_k' = U_k \Sigma_k' V_k^T, \quad k = 1, 2, \ldots, s,$$  \hfill (18)

to $A'$, where $U_k = (u_1, \ldots, u_k), V_k = (v_1, \ldots, v_k)$ and $\Sigma_k' = \text{diag}(\sigma_1, \ldots, \sigma_k)$ because $x_k^{\text{tsvd}} = A_i^T b = (A_i')^T b$.

With the above analysis and simple justifications, we can present the following theorem.

**Theorem 2.1.** Let $A_k, A'$ and $A_k'$ be defined by (9), (16) and (18). Then for $k = 1, 2, \ldots, s$ the TSVD solutions $x_k^{\text{tsvd}}$ satisfy

$$x_k^{\text{tsvd}} = A_i^T b = (A_i')^T b,$$  \hfill (19)

$$\|Ax_k^{\text{tsvd}} - b\| = \|A_kx_k^{\text{tsvd}} - b\| = \|A_k'x_k^{\text{tsvd}} - b\| = \|A'x_k^{\text{tsvd}} - b\|.$$  \hfill (20)

Particularly, for $k = s$, we have

$$x_{\text{naive}} = x_s^{\text{tsvd}} = A^T b = (A')^T b.$$  \hfill (21)
The above results show that solving (8) amounts to solving the problem

\[
\min \| x \| \quad \text{subject to} \quad \| A'_k x - b \| = \min
\]

for the same \( k \) and that (8) and (22) have the same solutions and residual norms for \( k = 1, 2, \ldots, s \).

**Remark 2.1.** Relations (19)–(22) mean that the TSVD method computes the same TSVD regularized solutions \( x_{\text{tsvd}}^k \), \( k = 1, 2, \ldots, s \), to (1) and the modified problem

\[
\min_{x \in \mathbb{R}^n} \| A' x - b \|
\]

and generates the same residuals for (1) and (23). For \( L = I \), the analogues of the regularization problems (3) and (4) corresponding to problem (23) now replace \( A \) by \( A' \). Relation (13) or (14) states that problem (23) satisfies the discrete Picard condition. We remind that the regularization parameter \( k \) of the TSVD method for solving (23) corresponds to the regularization parameter \( c_1 + c_2 + \cdots + c_k \) in (8) for solving (1).

The covariance matrix of the Gaussian white noise \( e \) is \( \eta^2 I \), and the expected value \( \mathcal{E}(\| e \|^2) = m \eta^2 \). With the SVD (16) of \( A' \), it holds that \( \mathcal{E}(\| u_i^T e \|) = \eta_i, \ i = 1, 2, \ldots, s \), and \( \| e \| \approx \sqrt{m \eta} \) and \( |u_i^T e| \approx \eta_i, \ i = 1, 2, \ldots, s \); see, e.g., [23, pp 70–71] and [25, pp 41–42]. The noise \( e \) thus affects \( u_i^T b, \ i = 1, 2, \ldots, s \), more or less equally. Relation (14) shows that for large singular values \( |u_i^T b_{\text{true}}|/\sigma_i \) is dominant relative to \( |u_i^T e|/\sigma_i \). Once \( |u_i^T b_{\text{true}}| \leq |u_i^T e| \) from some \( i \) onwards, the small singular values magnify \( |u_i^T e|/\sigma_i \), and the noise \( e \) dominates \( |u_i^T b|/\sigma_i \) and must be suppressed. The transition point \( k_0 \) is such that

\[
|u_i^T b| \approx |u_i^T b_{\text{true}}| > |u_i^T e| \approx \eta_i, \ |u_i^T b_{k_0+1}| \approx |u_i^T b_{k_0+1}| \approx \eta_i;
\]

see [25, pp 42, 98] and a similar description [23, pp 70–71]. In this sense, the \( \sigma_k \) are divided into the \( k_0 \) large and \( s - k_0 \) small ones. The TSVD solutions

\[
x_{\text{tsvd}}^k = \begin{cases} \sum_{i=1}^{k_0} \frac{u_i^T b}{\sigma_i} v_i \approx \sum_{i=1}^{k_0} \frac{u_i^T b_{\text{true}}}{\sigma_i} v_i, & k \leq k_0; \\ \sum_{i=1}^k \frac{u_i^T b}{\sigma_i} v_i \approx \sum_{i=1}^{k_0} \frac{u_i^T b_{\text{true}}}{\sigma_i} v_i + \sum_{i=k_0+1}^k \frac{u_i^T e}{\sigma_i} v_i, & k_0 < k \leq s. \end{cases}
\]

It is easily justified from [23, pp 70–71] and [25, pp 71, 86–88, 96] that \( x_{\text{tsvd}}^k \) first converges to \( x_{\text{true}} \) and the error \( \| x_{\text{true}} - x_{\text{tsvd}}^k \| \) and the residual norm \( \| A' x_{\text{tsvd}}^k - b \| = \| A'_k x_{\text{tsvd}}^k - b \| \) monotonically decrease until \( \| A' x_{\text{tsvd}}^k - b \| \approx \| e \| \) for \( k = k_0 \), afterwards \( x_{\text{tsvd}}^k \) diverges and instead converges to \( x_{\text{naive}} \), while the residual norm \( \| A' x_{\text{tsvd}}^k - b \| = \| A'_k x_{\text{tsvd}}^k - b \| \) stabilizes for \( k \) not close to \( s \). Therefore, the index \( k \) plays the role of the regularization parameter, \( x_{\text{tsvd}}^k \) exhibits typical semi-convergence at \( k = k_0 \), and the best regularized solution \( x_{\text{tsvd}}^k = (A'_k)^+ b \) has minimum two-norm error.

For \( \hat{U} = (\hat{U}_1, \hat{U}_2, \ldots, \hat{U}_s) \) and \( \hat{V} = (\hat{V}_1, \hat{V}_2, \ldots, \hat{V}_s) \) defined in (12), recall that the first columns of \( \hat{U}_i \) and \( \hat{V}_i \) are \( u_i \) and \( v_i \), respectively, and \( b \) is orthogonal to the other columns of \( \hat{U}_i, \ i = 1, 2, \ldots, s \). Then it is straightforward to obtain

\[
\frac{\hat{V}_i \hat{U}_i^T b}{\sigma_i} = \frac{u_i^T b}{\sigma_i} v_i, \quad i = 1, 2, \ldots, s.
\]
Keep definition (16) of $A'$ in mind and remember the fact that $b$ is orthogonal to $U_\perp$ with $U = (u_1, u_2, \ldots, u_s, U_\perp)$ in (16). Therefore, it follows from (4), (12) and (26) that, for a given parameter $\lambda$, the solution $x_\lambda$ of the Tikhonov regularization problem (4) is

$$
x_\lambda = (A^T A + \lambda^2 I)^{-1} A^T b = \sum_{i=1}^{s} f_i \tilde{V}_i^T \tilde{u}_i / \sigma_i
$$

(27)

$$
= \sum_{i=1}^{s} f_i \tilde{V}_i^T \tilde{u}_i = ((A')^T A' + \lambda^2 I)^{-1} (A')^T b,
$$

(28)

where the filters $f_i = \sigma_i^2 / (\sigma_i^2 + \lambda^2)$, $i = 1, 2, \ldots, s$. Therefore, $x_\lambda$ is a filtered SVD expansion of $A'$. Relations (27) and (28) have proved the following basic result.

**Theorem 2.2.** For the same $\lambda > 0$, problem (4) with $L = I$ is equivalent to the standard-form Tikhonov regularization

$$
\min_{x \in \mathbb{R}^n} \{ \| A' x - b \|^2 + \lambda^2 \| x \|^2 \}
$$

(29)

of the modified problem (23).

$x_{\text{SVD}}^\text{true}$ by the TSVD method is a special filtered SVD expansion, where $f_i = 1, i = 1, 2, \ldots, k$ and $f_i = 0, i = k + 1, \ldots, s$. The best Tikhonov regularized solution $x_{\text{opt}}$, which is defined as $\| x_{\text{true}} - x_{\text{opt}} \| = \min_{\lambda \geq 0} \| x_{\text{true}} - x_\lambda \|$, retains the $k_0$ dominant SVD components of $A'$ and dampens the other $s - k_0$ small SVD components as much as possible. The semi-convergence of the Tikhonov regularization method occurs at $\lambda_{\text{opt}}$ when the parameter $\lambda$ varies from zero to infinity.

Finally, we stress that our above changes and reformulations are purely for a mathematical analysis, which aims to extend the results in [33, 34] to the multiple singular value case. Computationally, we never need to reorganize the SVD of $A$ and construct $A'$ explicitly. Our conclusion is that solving (3) by the TSVD method and the Tikhonov regularization method is mathematically equivalent to solving (23) *implicitly* by these two methods. However, regarding the explicit construction of $U_\perp$, $V_i$ from $U$ and $V$, separately, though it is unnecessary in this paper, as we have pointed out, we have proposed two efficient and reliable construction procedures, which may have potentials in some other contexts.

### 3. The LSQR algorithm

The LSQR algorithm is based on Golub–Kahan bidiagonalization, algorithm 1, 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 $K_{k+1}(A A^T, b)$ for $k = 1, 2, \ldots, n$, respectively. We will prove that solving (3) by LSQR mathematically amounts to solving (23) *implicitly* by LSQR without forming $A'$ in (23), that is, LSQR works on (3) exactly as if it implicitly works on (23). Precisely, this implies that we only need to consider LSQR for (23) and all the results that hold for $A'$ and the modified problem (23) exactly reflect the regularization behavior of LSQR for the original problem (3) when $A$ has multiple singular value(s), as will be clear later.

From algorithm 1, we obtain the following relations:

$$
A Q_k = P_{k+1} B_k,
$$

(30)

$$
A^T P_{k+1} = Q_k B^T_k + \alpha_k q_{k+1} s^{(k+1)}_{k+1} T,
$$

(31)
Algorithm 1. k-step Golub–Kahan bidiagonalization process.

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

where $e^{(k+1)}_{k+1}$ is the $(k+1)$th canonical basis vector of $\mathbb{R}^{k+1}$, $P_{k+1} = (p_1, p_2, \ldots, p_{k+1})$, $Q_k = (q_1, q_2, \ldots, q_k)$, and

$$B_k = \begin{pmatrix} \alpha_1 & \beta_2 & \alpha_2 & \cdots \\ \beta_2 & \alpha_3 & \cdots \\ \alpha_3 & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \beta_{k+1} & \end{pmatrix} \in \mathbb{R}^{(k+1)\times k}. \quad (32)$$

It follows from (30) that

$$B_k = P_{k+1}^T A Q_k. \quad (33)$$

We remind that 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, provided that algorithm 1 does not break down until step $k$.

At iteration $k$, LSQR solves the problem

$$\|Ax_{\text{lsqr}}^k - b\| = \min_{x \in \mathbb{R}^n} \|Ax - b\|$$

and computes the iterate $x_{\text{lsqr}}^k = Q_k y_{\text{lsqr}}^k$ with

$$y_{\text{lsqr}}^k = \arg\min_{y \in \mathbb{R}^k} \|B_k y - \beta_1 e^{(k+1)}_{1}\| = \beta_1 B_k^\dagger e^{(k+1)}_{1}, \quad (34)$$

where $e^{(k+1)}_{1}$ is the first canonical basis vector of $\mathbb{R}^{k+1}$, and the solution norm $\|x_{\text{lsqr}}^k\| = \|y_{\text{lsqr}}^k\|$ increases and the residual norm $\|Ax_{\text{lsqr}}^k - b\| = \|B_k y_{\text{lsqr}}^k - \beta_1 e^{(k+1)}_{1}\|$ decreases monotonically with respect to $k$. From $\beta_1 e^{(k+1)}_{1} = P_{k+1}^T b$ and (34), we obtain

$$x_{\text{lsqr}}^k = Q_k B_k^\dagger P_{k+1}^T b, \quad (35)$$

which solves the problem

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

Next we will prove that algorithm 1 and LSQR work exactly as if they are applied to $A'$ and (23), that is, they generate the same results when applied to solving problems (1) and (23).

By (17), let us expand $b$ as

$$b = U_s U_s^T b + (I - U_s U_s^T) b = \sum_{j=1}^s \xi_j u_j + (I - U_s U_s^T) b.$$ 

12
By the SVD (12) of $A$ and the SVD (16) of $A'$ as well as the description on them, it is straightforward to justify that

$$K_k(A^TA, A^Tb) = K_k((A')^TA', (A')^Tb)$$

(36)

and

$$K_k(AA^T, b) = K_k(A'(A')^T, b)$$

(37)

by noting that

$$(A^TA)^iA^Tb = (A'^T)^i(A'^Tb) = \sum_{j=1}^{s} \xi_j \sigma_j^{2i+1} v_j$$

(38)

for any integer $i \geq 0$ and

$$(AA^T)^i b = (A'(A')^T)^i b = \sum_{j=1}^{s} \xi_j \sigma_j^{2i} u_j$$

(39)

for any integer $i \geq 1$. Thus, for the given $b$, algorithm 1 works on $A$ exactly as if it does on $A'$, that is, (30)–(33) hold when $A$ is replaced by $A'$. As a result, the $k$ distinct Ritz values $\theta_k^{(k)}$ approximate $k$ nonzero singular values of $A'$, i.e., $k$ distinct singular values of $A$. Particularly, from (33) we have

$$B_k = P_{s+1}^T A' Q_s.$$

(40)

Moreover, (38) and (39) show

$$K_{k+1}(A'^TA', (A')^Tb) = K_{k+1}((A')^TA', (A')^Tb), \quad K_{k+1}(A'(A')^T, b) = K_{k+1}(A'(A')^T, b).$$

As a result, since $(A')^T b$ has nonzero components in all the right singular vectors $v_1, v_2, \ldots, v_s$ of $A'$ associated with its nonzero distinct singular values $\sigma_1, \sigma_2, \ldots, \sigma_s$, Golub–Kahan bidiagonalization cannot break down until step $s$, and the $s$ singular values $\theta_j^{(s)}$ of $B_s$ are exactly the singular values $\sigma_1, \sigma_2, \ldots, \sigma_s$ of $A'$. At step $s$, Golub–Kahan bidiagonalization generates the orthonormal $P_{s+1}, Q_s$ and the matrix $1$

$$P_{s+1}^T A Q_s = P_{s+1}^T A' Q_s = B_s.$$

(41)

and

$$\text{span}\{V_s\} = \text{span}\{Q_s\}, \quad \text{span}\{U_s\} \subset \text{span}\{P_{s+1}\}.$$

(42)

Since (30)–(33) hold when $A$ is replaced by $A'$, LSQR works exactly as if it solves (23), similarly to the TSVD method (cf (22)). However, there is a remarkable difference between LSQR and the TSVD method in the multiple singular value case: LSQR applied to (1) and (23) generates exactly the same results at the same iteration $k$, while the the TSVD method applied to (23) at the regularization parameter $k$ generates the same results as the TSVD method applied to (1) does at the regularization parameter $c_1 + c_2 + \cdots + c_k$.

1If $m = n$, it is easily justified that $\beta_{s+1} = 0$, algorithm 1 produces the orthonormal matrices $P_s, Q_s$ and the $s \times s$ lower bidiagonal $B_s$ with the positive diagonals $\alpha_i$ and subdiagonals $\beta_i$. This does not affect all the derivation and results followed, and we only need to replace $P_{s+1}$ by $P_s$. For example, $\text{span}\{U_s\} = \text{span}\{P_s\}$ in (42).
We summarize the results on LSQR as follows.

**Theorem 3.1.** The LSQR iterate $x_{k}^{\text{lsqr}}$ is the solution to the problem
\begin{equation}
\min \|x\| \quad \text{subject to} \quad \|P_{k+1}\bar{B}_k\bar{Q}_k^Tx - b\| = \min
\end{equation}
starting with $k = 1$ onwards, and it is a regularized solution of problem (23) and problem (1) and satisfies
\begin{equation}
\|Ax_{k}^{\text{lsqr}} - b\| = \|A'x_{k}^{\text{lsqr}} - b\| = \|B_{k}x_{k}^{\text{lsqr}} - \beta_{1}^{(k+1)}\|, \quad k = 1, 2, \ldots, s
\end{equation}
with $x_{k}^{\text{lsqr}}$ defined by (34).

The rank $k$ approximation $P_{k+1}\bar{B}_k\bar{Q}_k^T$ to $A'$ in (43) plays a role similar to the best rank $k$ approximation $A'_k$ to $A'$ in (22). Recall that the best rank $k$ approximation $A'_k$ to $A'$ satisfies $\|A' - A'_k\| = \sigma_{k+1}$. For the rank $k$ approximation $P_{k+1}\bar{B}_k\bar{Q}_k^T$ to $A'$ in LSQR, we define
\begin{equation}
\gamma_{k}^l = \|A' - P_{k+1}\bar{B}_k\bar{Q}_k^T\|, \quad k = 1, 2, \ldots, s - 1,
\end{equation}
which measures the accuracy of the rank $k$ approximation $P_{k+1}\bar{B}_k\bar{Q}_k^T$ to $A'$. The rank $k$ matrix $P_{k+1}\bar{B}_k\bar{Q}_k^T$ is called a near best rank $k$ approximation to $A'$ if it satisfies
\begin{equation}
\sigma_{k+1} \leq \gamma_{k}^l < \frac{\sigma_k + \sigma_{k+1}}{2},
\end{equation}
that is, $\gamma_{k}^l$ lies between $\sigma_{k+1}$ and $\sigma_k$ and is closer to $\sigma_{k+1}$. This definition has been introduced in [34] and shown to be irreplaceable in the context of linear discrete ill-posed problems when considering the approximation behavior of the Ritz values $\theta_i^{(k)}$ and the counterparts involved in the Krylov solvers CGME and LSMR [35].

LSQR has the same regularization ability as the TSVD method and thus has the full regularization if (i) $P_{k+1}\bar{B}_k\bar{Q}_k^T$ is a near best rank $k$ approximation to $A'$ with an approximate accuracy $\sigma_{k+1}$ and (ii) the $k$ singular values of $B_k$ approximate the first $k$ large ones of $A'$ in natural order for $k = 1, 2, \ldots, k_0$, that is, they interlace the first $k + 1$ large $\sigma_i$ for $k = 1, 2, \ldots, k_0$. The fact that LSQR definitely has the full regularization under these two conditions is clearly trivial: (i) $x_k^{\text{svd}}$ and $x_k^{\text{lsqr}}$ are the regularized solutions to the two perturbed problems of (23) that replace $A'$ by the two rank $k$ approximations with the same quality to $A'$, respectively; (ii) $x_k^{\text{svd}}$ and $x_k^{\text{lsqr}}$ solve the two essentially same regularization problems (22) and (43), respectively. Therefore, the near best rank $k$ approximation of $P_{k+1}\bar{B}_k\bar{Q}_k^T$ to $A'$ and the approximations of the $k$ singular values of $B_k$ to the large ones of $A'$ in natural order for $k = 1, 2, \ldots, k_0$ are sufficient conditions for LSQR to have the full regularization. However, one must be well aware that they are not necessary conditions for the full regularization of LSQR, as has been specially stressed and numerically justified in [33, 34].

4. $\sin \Theta$ theorems for the distances between $K_k((A')^TA', (A')^Tb)$ and the dominant right singular subspace span $\{V_k\}$

In the multiple singular value case, based on the work in sections 2 and 3, just as [33, 34], under the discrete Picard condition (14), a complete understanding of the regularization of LSQR includes accurate solutions of the following problems: (i) how accurately does $K_k((A')^TA', (A')^Tb)$ approximate the $k$ dimensional dominant right singular subspace span $\{V_k\}$ of $A'$ spanned by the columns of $V_k = (v_1, v_2, \ldots, v_k)$? (ii) How accurate is the rank $k$ approximation $P_{k+1}\bar{B}_k\bar{Q}_k^T$ to $A'$? (iii) When do the $k$ Ritz values $\theta_i^{(k)}$ approximate the the first $k$ large $\sigma_i$
in natural order? (iv) When does at least a small Ritz value appear, i.e., \( \theta^{(k)}_k < \sigma_{k+1} \) for some \( k \leq k' \) with \( k' \) the iteration at which the semi-convergence of LSQR occurs? (v) Does LSQR have the full or partial regularization when the \( k \) Ritz values \( \theta^{(k)}_k \) do not approximate the large singular values of \( A \) in natural order for some \( k \leq k' \)?

We will focus on problems (i)–(iv) and extend all the results in [33, 34] to the multiple singular value case. On the other hand, as one of the main contributions, we will make a novel general analysis that covers but is not limited to problem (iii) and (iv) and get more insight into them when \( A \) has simple or multiple singular values.

Based on a well-known result (see e.g., van der Sluis and van der Vorst [51, property 2.8]), it is straightforward to establish the following result, which, based on the work of section 3, holds when \( A \) is replaced by \( A' \), and has been used in Hansen [23] and the references therein as well as in [33] to illustrate the regularizing effects of LSQR.

**Proposition 4.1.** LSQR with the starting vector \( p_1 = b / \| b \| \) and CGLS applied to the normal equation \( (A')^TA'x = (A')^Tb \) of (23) with the zero starting vector generate the same iterates

\[
x_{k}^{\text{lsqr}} = \sum_{i=1}^{s} f_i^{(k)} u_i^T b / \sigma_i v_i, \quad k = 1, 2, \ldots, s,
\]

(47)

where the filters

\[
f_i^{(k)} = 1 - \prod_{j=1}^{k} \left( \frac{(\theta_i^{(j)})^2 - \sigma_j^2}{(\theta_i^{(j)})^2} \right), \quad i = 1, 2, \ldots, s,
\]

(48)

and the \( \theta_i^{(k)} \) are the singular values of \( B_k \) labeled as \( \theta_1^{(k)} > \theta_2^{(k)} > \cdots > \theta_k^{(k)} \).

Relation (47) shows that \( x_k^{\text{lsqr}} \) has a filtered SVD expansion similar to (28). It is easily justified that if all the Ritz values \( \theta_i^{(k)} \) approximate the first \( k \) singular values \( \sigma_j \) of \( A' \) in natural order then \( f_i^{(k)} \approx 1 \), \( i = 1, 2, \ldots, k \) and the other \( f_i^{(k)} \) monotonically decreases and approaches zero with respect to \( i = k + 1, \ldots, s \) since the \( \sigma_i \) are labeled in decreasing order and supposed to approach zero as \( i \) increases. This indicates that if the \( \theta_i^{(k)} \) approximate the first \( k \) singular values \( \sigma_j \) of \( A' \) in natural order for \( k = 1, 2, \ldots, k_0 \) then \( x_k^{\text{lsqr}} \) is as accurate as \( x_k^{\text{svd}} \), meaning that LSQR has the full regularization and computes a best possible two-norm filtering regularized solution. Using the same proof as that of [33, theorem 3.1], we obtain the following basic results.

**Theorem 4.1.** The semi-convergence of LSQR must occur at some iteration

\[ k^* \leq k_0. \]

If the Ritz values \( \theta_i^{(k)} \) do not converge to the large singular values of \( A' \) in natural order for some \( k \leq k^* \), then \( k^* < k_0 \) strictly. On the other hand, if \( k^* < k_0 \), then the Ritz values \( \theta_i^{(k)} \) must not converge to the first \( k \) large singular values \( \sigma_j \) of \( A \) in natural order for some \( k \leq k^* \).

We must keep in mind that the semi-convergence point \( k_0 \) of the TSVD method for the modified problem (23) corresponds to the semi-convergence point \( c_1 + c_2 + \cdots + c_{k_0} \) of the TSVD method for the original problem (1). It implies that if the Ritz values \( \theta_i^{(k)} \) interface the first \( k + 1 \) singular values of \( A' \) from \( k = 1 \) to the point \( k' \) of semi-convergence of LSQR then \( k_0 = k' \) and the TSVD method finds the best possible regularized solution at step \( c_1 + c_2 + \cdots + c_{k_0} \) and \( \| A - A_{k_0} \| = \sigma_{k_0 + 1} \), where \( A_{k_0} \) is defined by (9). Therefore, in the multiple singular value
case, LSQR may use much fewer iterations to attain the semi-convergence than the TSVD method does when the $\theta^{(k)}_j$ approximate the first $k$ large singular values of $A'$ in natural order until semi-convergence. This is definitely true provided that there is (are) some $c_j$ multiple $\sigma_j$ with $j \leq k^*$ and $c_j > 1$ considerably.

The approximation accuracy of $P_{k+1}B_kQ^T_k$ to $A'$ and the approximation properties of $\theta^{(k)}_j$, $j = 1, 2, \ldots, k$, critically depend on how the underlying $k$ dimensional $K_k((A')^TA', (A')^Tb)$, from which the iterate $x^{(k)}_D$ is extracted, approximates the $k$ dimensional dominant right singular subspace $\text{span}\{V_k\}$ of $A'$. In terms of the canonical angles $\Theta(\mathcal{X}, \mathcal{Y})$ between two subspaces $\mathcal{X}$ and $\mathcal{Y}$ of equal dimension (see [49, pp 74–75] and [50, p 43]), we present the following general result, which is the same as lemma 4.1 in [33] except that $n$ is replaced by $s$. However, its proof is not directly available from that of [33] because $A'$ has an $n-s$ multiple zero singular value, so that we need to make some nontrivial changes to prove it.

**Lemma 4.1.** Let $\{V_k\} = K_k((A')^TA', (A')^Tb)$ and $V_k = \text{span}\{V_k\}$ with $V_k = (v_1, v_2, \ldots, v_k)$, the $k$-dimensional dominant right singular subspace of $A'$. Then for $k = 1, 2, \ldots, s-1$ we have

$$
\| \sin \Theta(V_k, V^R_k) \| = \frac{\| \Delta_k \|}{\sqrt{1 + \| \Delta_k \|^2}}
$$

(49)

with $\Delta_k \in \mathbb{R}^{(n-k)xk}$ defined by (51), i.e.,

$$
\| \tan \Theta(V_k, V^R_k) \| = \| \Delta_k \|.
$$

(50)

**Proof.** In order to prove (49), we need to make some nontrivial changes in the proof of lemma 4.1 in [33].

From (16), observe the Krylov subspace $K_k((\Sigma_j^T, \Sigma_j^T)U^Tb) = \text{span}\{\hat{D}T_k\}$ with

$$
\hat{D} = \text{diag}(\sigma_1u_1^Tb, \ldots, \sigma_su_s^Tb, 0) = \begin{pmatrix} D \\ 0 \end{pmatrix} \in \mathbb{R}^{n \times n}
$$

and

$$
\hat{T}_k = \begin{pmatrix}
1 & \sigma_1^2 & \ldots & \sigma_s^{2k-2} \\
1 & \sigma_2^2 & \ldots & \sigma_s^{2k-2} \\
\vdots & \vdots & \ddots & \vdots \\
1 & \sigma_s^2 & \ldots & \sigma_s^{2k-2} \\
0 & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & 0
\end{pmatrix} = \begin{pmatrix} T_k \\ 0 \end{pmatrix} \in \mathbb{R}^{n \times k}.
$$

Partition the diagonal matrix $D$ and the matrix $T_k$ as

$$
D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix} \in \mathbb{R}^{x \times x}, \quad T_k = \begin{pmatrix} T_{k1} \\ T_{k2} \end{pmatrix} \in \mathbb{R}^{x \times k},
$$

where $D_1, T_{k1} \in \mathbb{R}^{k \times k}$. Since $T_{k1}$ is a Vandermonde matrix with $\sigma_j$ distinct for $j = 1, 2, \ldots, k$, it is nonsingular. Therefore, from

$$
V^R_k = K_k((A')^TA', (A')^Tb) = \text{span}\{V^R \hat{D}T_k\}
$$
and the structures of $\hat{D}$ and $\hat{T}_k$ as well as (17), we obtain

$$\mathcal{V}_k^R = \text{span}\{V_k D T_k\} = \text{span}\left\{V_s \left( \begin{array}{c} D_1 T_{k1} \\ D_2 T_{k2} \end{array} \right) \right\} = \text{span}\left\{V_s \left( \begin{array}{c} I \\ \Delta_k \end{array} \right) \right\},$$

with

$$\Delta_k = D_2 T_{k2} T_{k1}^{-1} D_1^{-1},$$

meaning that $\mathcal{V}_k^R$ is orthogonal to $V_\perp$ in (17).

Recall (16) and write

$$V_k = (V_k, V_\perp),$$

whose columns are the right singular vectors of $A'$ associated with the nonzero singular values $\sigma_i, i = 1, 2, \ldots, s$. Define

$$Z_k = V_s \left( \begin{array}{c} I \\ \Delta_k \end{array} \right) = V_k + V_\perp \Delta_k.$$

Then $Z_k^2 Z_k = I + \Delta_k^2 \Delta_k$, and the columns of $\hat{Z}_k = Z_k (Z_k^T Z_k)^{-\frac{1}{2}}$ form an orthonormal basis of $\mathcal{V}_k^R$. Therefore, for $V_\perp$ defined in (17), whose columns are the right singular vectors of $A'$ associated with the $n - s$ multiple zero singular values, we have $V_\perp^T \hat{Z}_k = 0$ and obtain an orthogonal direct sum decomposition

$$\hat{Z}_k = (V_k + V_\perp \Delta_k)(I + \Delta_k^2 \Delta_k)^{-\frac{1}{2}}.$$ in $\mathbb{R}^n$. Based on the above, (17) and (52), by the definition of $\| \sin \Theta(V_\perp, \mathcal{V}_k^R) \|$ and $V_\perp^T \hat{Z}_k = 0$, we obtain

$$\| \sin \Theta(V_\perp, \mathcal{V}_k^R) \| = \| (V_k^\perp, V_\perp)^T \hat{Z}_k \| = \| \Delta_k (I + \Delta_k^2 \Delta_k)^{-\frac{1}{2}} \| = \frac{\| \Delta_k \|}{\sqrt{1 + \| \Delta_k \|}},$$

which proves (49). Relation (50) follows from (49) directly. \hfill \square

This theorem shows that $\mathcal{V}_k^R$ approximates the $k$-dimensional dominant right singular subspace $\mathcal{V}_k$ of $A'$ and that it makes no sense for $\mathcal{V}_k^R$ to approximate the $k$-dimensional dominant right singular subspace of $A$ itself in the multiple singular value case. It will turn out that the size of $\| \Delta_k \|$ plays a vital role in the approximation accuracy of $P_{k+1} B_k Q_k^T$ to $A'$ and the approximation behavior of the Ritz values $\theta_k^{(i)}, i = 1, 2, \ldots, k$; see later theorems 4.2, 5.1–5.3 and 6.1 as well as the analysis on them.

In the multiple singular value case, since problem (1) is equivalent to problem (23), problems (1) and (23) have the same degree of ill-posedness, which is decided by the decay rate of the singular values of $A'$. For the cases that problem (23) is severely, moderately and mildly ill-posed, that is, the $s$ nonzero singular values $\sigma_j = O(\rho^{-j})$ and $\sigma_j = \zeta^{-\alpha}$ of $A'$ with $\zeta > 0$ a constant and $\alpha > 1$ and $\frac{1}{2} < \alpha \leq 1$, respectively, all the estimates for $\| \Delta_k \|$ and analysis in [33] can be adapted to our context correspondingly without changes except that $n$ is replaced by $s$, and the proofs are directly applicable without modifications. Therefore, we do not repeat the results and instead refer the reader to theorems 4.2–4.5 in [33].

The author in [33] has investigated how $\| \sin \Theta(V_\perp, \mathcal{V}_k^R) \|$ affects the smallest Ritz value $\theta_k^{(i)}$ in the simple singular value case. In the case that $A$ has multiple singular value(s), since LSQR
works on (3) exactly as if it does on (23), we can establish the same results hold for \( A' \) by modifying the proof in [33] due to the occurrence of \( n - s \) multiple zero singular value in \( A' \). 

**Theorem 4.2.** Let \( \| \sin(\Theta(V_k, \mathbb{V}_k^R)) \|^2 = 1 - \varepsilon_k^2 \) with \( 0 < \varepsilon_k < 1 \), \( k = 1, 2, \ldots, s - 1 \), and \( \tilde{q}_k \in \mathbb{V}_k^R \) with \( \| \tilde{q}_k \| = 1 \) be the vector having the smallest angle with \( \text{span}\{V_k', V_\perp\} \) defined by (17) and (52), i.e., the orthogonal complement of \( \mathbb{V}_k \) with respect to \( \mathbb{R}^n \). Then it holds that

\[
e_k^2 \sigma_k^2 + (1 - \varepsilon_k^2)\sigma_n^2 < \tilde{q}_k(A'\tilde{q})_k < e_k^2 \sigma_{k+1}^2 + (1 - \varepsilon_k^2)\sigma_1^2.
\]

If \( \varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k} \), then

\[
\sqrt{q_k^T (A')^T A' q_k} > \sigma_{k+1};
\]

if \( \varepsilon_k^2 \leq \frac{\delta}{\sigma_k + \varepsilon_k} \) for a given arbitrarily small \( \delta > 0 \), then

\[
\theta^{(k)}_k < (1 + \delta)^{1/2} \sigma_{k+1},
\]

meaning that \( \theta^{(k)}_k < \sigma_{k+1} \) once \( \varepsilon_k \) is sufficiently small, i.e., \( \| \sin(\Theta(V_k, \mathbb{V}_k^R)) \| \) is sufficiently close to one.

**Proof.** Since the columns of \( Q_k \) generated by Golub–Kahan bidiagonalization form an orthonormal basis of \( \mathbb{V}_k^R \), by definition and the assumption on \( \tilde{q}_k \), we have

\[
\| \sin(\Theta(V_k, \mathbb{V}_k^R)) \| = \| (V_k^\perp, V_\perp)^T Q_k \| = \| (V_k^\perp, V_\perp)^T Q \|
\]

\[
= \max_{|e|=1} \| (V_k^\perp, V_\perp)^T Q e \|
\]

\[
= \| (V_k^\perp, V_\perp)^T Q_k e \|
\]

\[
= \| (V_k^\perp, V_\perp)^T \tilde{q}_k \|
\]

\[
= \| (V_k^\perp, V_\perp)^T \tilde{q}_k \| = \sqrt{1 - \varepsilon_k^2}
\]

(57)

with \( \tilde{q}_k = Q_k e_k \in \mathbb{V}_k^R \) and \( \| e_k \| = 1 \).

Notice that \( V = (V_k, V_k^\perp, V_\perp) \). Expand \( \tilde{q}_k \) as the following orthogonal direct sum decomposition:

\[
\tilde{q}_k = (V_k^\perp, V_\perp)(V_k^\perp, V_\perp)^T \tilde{q}_k + V_k V_k^T \tilde{q}_k.
\]

(58)

Then from \( \| \tilde{q}_k \| = 1 \) and (57) we obtain

\[
\| V_k^T \tilde{q}_k \| = \| V_k V_k^T \tilde{q}_k \|
\]

\[
= \sqrt{1 - \| (V_k^\perp, V_\perp)^T \tilde{q}_k \|^2} = \sqrt{1 - (1 - \varepsilon_k^2)} = \varepsilon_k.
\]

(59)

We next bound the Rayleigh quotient of \( (A')^T A' \) with respect to \( \tilde{q}_k \) from below. By \( A' = U\Sigma' V^T \) defined in (16) and (52), we partition

\[
\Sigma' = \begin{pmatrix} \Sigma'_k & \Sigma'_{k,\perp} \\ 0 & 0 \end{pmatrix},
\]

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where $\Sigma_{k} = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_k)$ and $\Sigma_{k+1} = \text{diag}(\sigma_{k+1}, \sigma_{k+2}, \ldots, \sigma_s)$. Making use of $(A')'A'V_k = V_k(\Sigma_{k+1}')^2$, $(A')'A'V_k = V_k(\Sigma_{k+1})^2$ and $(A')'A'V_{\perp} = 0$ as well as $V_k^T V_k = 0$, $V_{\perp}^T V_{\perp} = 0$ and $V_k^T V_{\perp} = 0$, from (58) we obtain

$$
\bar{q}_k^T (A')'A' \bar{q}_k = (\hat{q}_k^T V_k^T (V_k^T)^T + \hat{q}_k^T V_{\perp} V_{\perp}^T + \hat{q}_k^T V_k^T V_k^T)
\times (V_k^T (\Sigma_{k+1}')^2 (V_k^T)^T \hat{q}_k + V_k (\Sigma_{k}^2)^2 V_k^T \hat{q}_k)
= \hat{q}_k^T V_k^T (\Sigma_{k+1}')^2 (V_k^T)^T \hat{q}_k + \hat{q}_k^T V_k (\Sigma_{k}^2)^2 V_k^T \hat{q}_k.
$$

(60)

It is impossible for $(V_k^T)^T \hat{q}_k$ and $V_k^T \hat{q}_k$ to be the eigenvectors of $(\Sigma_{k+1}')^2$ and $(\Sigma_{k}^2)^2$ associated with their respective smallest eigenvalues $\sigma_{k+1}^2$ and $\sigma_{k}^2$ simultaneously, which are the $(s - k)$th canonical vector $e_{s-k}^{(56)}$ of $\mathbb{R}^s$ and the $k$th canonical vector $e_{s-k}^{(56)}$ of $\mathbb{R}^s$, respectively; otherwise, we have $\hat{q}_k = v_k$ and $\hat{q}_k = v_k$ simultaneously, which are impossible as $v_k$ and $v_k$ are orthogonal for $k < s$. Therefore, from (60), (57) and (59), we obtain the strict inequality

$$
\bar{q}_k^T (A')'A' \bar{q}_k \geq \| (V_k^T)^T \hat{q}_k \|^2 \sigma_{k}^2 + \| V_k^T \hat{q}_k \|^2 \sigma_{k+1}^2 = (1 - \varepsilon_k^2) \sigma_{k}^2 + \varepsilon_k^2 \sigma_{k+1}^2,
$$

from which it follows that the lower bound of (54) holds.

Similarly, from (60), (57) and (59) we obtain the upper bound of (54):

$$
\bar{q}_k^T (A')'A' \bar{q}_k \leq \| (V_k^T)^T \hat{q}_k \|^2 \| (\Sigma_{k+1}')^2 \| + \| V_k^T \hat{q}_k \|^2 \| (\Sigma_{k}^2)^2 \| = (1 - \varepsilon_k^2) \sigma_{k+1}^2 + \varepsilon_k^2 \sigma_{k+1}^2.
$$

From the lower bound of (54), we see that if $\varepsilon_k$ satisfies $\varepsilon_k^2 \sigma_k^2 \geq \sigma_{k+1}^2$, i.e., $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$, then $\sqrt{\bar{q}_k^T (A')'A' \bar{q}_k} > \sigma_{k+1}$, i.e., (55) holds.

Recall from section 3 that algorithm 1 generates the same results when applied to $A$ and $A'$. Therefore, from (40), we obtain $B_k^T B_k = \hat{Q}_k^T (A')'A' \hat{Q}_k$. Since $(\theta_k^{(56)})^2$ is the smallest eigenvalue of the symmetric positive definite matrix $B_k^T B_k$, we have

$$
(\theta_k^{(56)})^2 = \min_{\|c\|_1 = 1} c^T \hat{Q}_k^T (A')'A' \hat{Q}_k c
= \min_{\hat{q} \in \mathbb{R}^s, \|\hat{q}\|_1 = 1} \hat{q}^T (A')'A' \hat{q} = \bar{q}_k^T (A')'A' \bar{q}_k.
$$

(61)

Therefore, for $\hat{q}_k$, we have

$$
\theta_k^{(56)} \leq \sqrt{\bar{q}_k^T (A')'A' \bar{q}_k},
$$

from which it follows from (54) that $(\theta_k^{(56)})^2 < (1 - \varepsilon_k^2) \sigma_{k+1}^2 + \varepsilon_k^2 \sigma_{k}^2$. As a result, for any $\delta > 0$, we can choose $\varepsilon_k \geq 0$ such that

$$
(\theta_k^{(56)})^2 < (1 - \varepsilon_k^2) \sigma_{k+1}^2 + \varepsilon_k^2 \sigma_{k}^2 \leq (1 + \delta) \sigma_{k+1}^2,
$$

i.e., (56) holds, solving which for $\varepsilon_k^2$ gives $\varepsilon_k^2 \leq \frac{\delta}{\sigma_{k+1}^2 - 1}$. \( \square \)

**Remark 4.1.** The author in [34] has made an analysis on $\| \sin \Theta (V_k, V_k^T) \|$ for the three kinds of ill-posed problems where singular values are all simple. The results show that $\| \sin \Theta (V_k, V_k^T) \|$ cannot be close to one for severely or moderately ill-posed problems with suitable $\rho > 1$ or $\alpha > 1$ and $k \leq k_0$, but it generally approaches one for mildly ill-posed problems or moderately ill-posed problems with $\alpha > 1$ but close to one when $k$ is small.
Remark 4.2. It has been shown in [34] that for severely and moderately ill-posed problems with suitable $\rho > 1$ and $\alpha > 1$, we may have $\theta_k^{(k)} > \sigma_{k+1}$ for $k \leq k^*$, and for mildly ill-posed problems and moderately ill-posed problems with $\alpha > 1$ but close to one we have $\theta_k^{(k)} < \sigma_{k+1}$ for some $k \leq k^*$.

Theorem 4.2 does not give any sufficient conditions on $\rho$ and $\alpha$ that ensures $\theta_k^{(k)} > \sigma_{k+1}$. In the next section, we present accurate results on problems (i)–(iv) stated in the beginning of section 4.

5. The rank $k$ approximation $P_{k+1}B_kQ_k^T$ to $A'$, the Ritz values $\theta_j^{(k)}$ and the regularization of LSQR

In this section, we present the results on the approximation accuracy of the rank $k$ approximation $P_{k+1}B_kQ_k^T$ to $A'$ and the convergence behavior of the Ritz values $\theta_j^{(k)}$, and draw some definitive conclusions on the regularization ability of LSQR for (23) and thus (1). These results, though their proofs are straightforward from the corresponding ones in [34], and some quantities and notation play a central role in section 7 and will be frequently exploited; the relationships between them and the TSVD method applied to problem (1) deserve special attention and numerical justifications. We will give some necessary explanations and address some special features of the results in the multiple singular value case. In fact, for the completeness of the regularization theory of LSQR in the multiple singular value case and for the readability of the paper, we should state them in order to make the paper self-contained.

Theorem 5.1. Assume that the discrete Picard condition (14) is satisfied, and define

$$
L_{b,i}^{(k)} = \max_{j=1,\ldots,k} L_{b,j}^{(k)}, \quad L_{j}^{(k)} = \prod_{i=1,|i|\neq j}^{k} \frac{\sigma_i^2}{|\sigma_j - \sigma_i|^2}, \quad j = 1, 2, \ldots, k
$$

(62)

with the definition $L_1^{(1)} = 1$. Then for $k = 1, 2, \ldots, s - 1$ we have

$$
\sigma_{k+1} \leq \gamma_k^{(k)} \leq \sqrt{1 + \eta_k} \sigma_{k+1}
$$

(63)

with

$$
\eta_k \leq \xi_k \frac{\max_{1 \leq j \leq k}|u_j^T b|}{\min_{1 \leq j \leq k}|u_j^T b|} \left(1 + O(\rho^{-2})\right), \quad k = 1, 2, \ldots, k_0
$$

(64)

for severely ill-posed problems with $\sigma_i = O(\rho^{-i})$, $i = 1, 2, \ldots, s$ and

$$
\eta_k \leq \begin{cases} 
\xi_1 \frac{\sigma_1}{\sigma_2} \frac{\max_{2 \leq j \leq k}|u_j^T b|}{|u_1^T b|} \sqrt{\frac{1}{2\alpha - 1}} & \text{for } k = 1, \\
\xi_k \frac{\sigma_k}{\sigma_{k+1}} \frac{\max_{k+1 \leq j \leq k}|u_j^T b|}{\min_{1 \leq j \leq k}|u_j^T b|} \sqrt{\frac{k^2}{4\alpha^2 - 1} + \frac{k}{2\alpha - 1} L_{k_1}^{(k)}} & \text{for } 1 < k \leq k_0
\end{cases}
$$

(65)

for moderately or mildly ill-posed problems with $\sigma_j = \zeta_j^{1/\alpha}$, $j = 1, 2, \ldots, s$, where $\xi_k = \sqrt{\left(\frac{\|b\|}{\|u_1\|\Delta b}\right)^2 + 1}$ for $\|\Delta b\| < 1$ and $\xi_k = \frac{\pi}{2\pi}$ for $\|\Delta b\| \geq 1$. 


Based on theorem 5.1, for the ill-posed problems with the singular value models \( \sigma_k = \zeta \rho^{-k} \) and \( \sigma_k = \zeta k^{-\alpha} \), the following two theorems establish the sufficient conditions on \( \rho \) and \( \alpha \) that guarantee that \( P_{k+1} B_k Q_k^T \) is a near best rank \( k \) approximation to \( A' \) and the Ritz values \( \theta_i^{(k)} \) approximate the \( k \) large singular values \( \sigma_i \) of \( A' \) in natural order for \( k = 1, 2, \ldots, k^* \), whose proofs are the same as those of theorems 3.3 and 4.1 in [34].

**Theorem 5.2.** Assume that the discrete Picard condition (14) is satisfied. Then, in the sense of (46), \( P_{k+1} B_k Q_k^T \) is a near best rank \( k \) approximation to \( A' \) if

\[
\sqrt{1 + \eta_k^2} < \frac{1}{2} \frac{\sigma_k}{\sigma_{k+1}} + \frac{1}{2}, \quad k = 1, 2, \ldots, k^*.
\]  

(66)

Furthermore, \( P_{k+1} B_k Q_k^T \) is a near best rank \( k \) approximation to \( A' \) if \( \rho > \frac{1 + \sqrt{2}}{2} \) for the severely ill-posed problems with \( \sigma_k = \zeta \rho^{-k} \) or \( \alpha \) satisfies

\[
2\sqrt{1 + \eta_k^2} - 1 < \left( \frac{k + 1}{k} \right)^{\alpha}, \quad k = 1, 2, \ldots, k^*
\]  

(67)

for the moderately and mildly ill-posed problems with \( \sigma_k = \zeta k^{-\alpha} \), respectively.

We must remind that in the multiple singular value case it is impossible for \( P_{k+1} B_k Q_k^T \) to be a good approximation to the original \( A \) whenever at least one of the first \( k \) nonzero singular values \( \sigma_k \) of \( A' \) is a multiple one of \( A \).

The author in [34] has analyzed this theorem; see remarks 3.8 and 3.9 there. It has been proved that, for severely and moderately ill-posed problems with suitable \( \rho > 1 \) and \( \alpha > 1 \), algorithm 1 always generates near best rank \( k \) approximations for \( k = 1, 2, \ldots, k^* \) but \( P_{k+1} B_k Q_k^T \) may not be a near best rank \( k \) approximation for moderately ill-posed problems with \( \alpha > 1 \) but close to one and mildly ill-posed problems for some \( k \leq k^* \).

**Theorem 5.3.** Assume that (23) is severely ill-posed with \( \sigma_i = \zeta \rho^{-i} \) and \( \rho > 1 \) or moderately ill-posed with \( \sigma_i = \zeta i^{-\alpha} \) and \( \alpha > 1 \), \( i = 1, 2, \ldots, s \), and the discrete Picard condition (14) is satisfied. Let the Ritz values \( \theta_i^{(k)} \) be labeled as \( \theta_1^{(k)} > \theta_2^{(k)} > \cdots > \theta_s^{(k)} \). Then

\[
\sigma_i - \theta_i^{(k)} \leq \gamma_k' \leq \sqrt{1 + \eta_k^2} \sigma_{k+1}, \quad i = 1, 2, \ldots, k.
\]  

(68)

For \( k = 1, 2, \ldots, k^* \), if \( \rho \geq 1 + \frac{\sqrt{2}}{2} \) or \( \alpha > 1 \) satisfies

\[
1 + \sqrt{1 + \eta_k^2} < \left( \frac{k + 1}{k} \right)^{\alpha},
\]  

(69)

then the \( \theta_i^{(k)} \) strictly interlace the first large \( k + 1 \) singular values of \( A' \) and approximate the first \( k \) large ones in natural order:

\[
\sigma_{i+1} < \theta_i^{(k)} < \sigma_i, \quad i = 1, 2, \ldots, k.
\]  

(70)

By applying the analysis in [34] to this theorem, we conclude that for severely and moderately ill-posed problems with suitable \( \rho > 1 \) and \( \alpha > 1 \), the \( \theta_i^{(k)} \) approximate the first \( k \) large singular values \( \sigma_i \) of \( A' \) in natural order until the semi-convergence of LSQR for severely and moderately ill-posed problems with suitable \( \rho > 1 \) and \( \alpha > 1 \), and such approximations in natural order generally fail for moderately ill-posed problems with \( \alpha > 1 \) but close to one and mildly ill-posed problems at some iterations \( k \leq k^* \). As a result, in the multiple singular value case, LSQR has the full regularization for severely and moderately ill-posed problems with suitable \( \rho > 1 \) and \( \alpha > 1 \).
6. Monotonicity of $\gamma_k'$ and decay rates of entries $\alpha_k$ and $\beta_{k+1}$ in $B_k$

In this section, we establish the results on the monotonicity of $\gamma_k'$ (cf (45)), derive the decay rates of $\alpha_k$ and $\beta_{k+1}$ in [34], and extend theorem 5.1 in [34] to the multiple singular value case. The proof path follows that of theorem 5.1 in [34] but need some nontrivial changes because, unlike the case that the singular values of $A$ are all simple, algorithm 1 cannot be run completion in the multiple singular value case.

**Theorem 6.1.** With the notation defined previously, the following results hold:

\[
\sqrt{\alpha_{k+1}^2 + \beta_{k+2}^2} < \gamma_k' \leq \sqrt{1 + \eta_k^2 \sigma_{k+1}}, \quad k = 1, 2, \ldots, s - 1,
\]

(71)

\[
\alpha_{k+1} \beta_{k+2} \leq \frac{(\gamma_k')^2}{2} \leq \frac{(1 + \eta_k^2) \sigma_{k+1}^2}{2}, \quad k = 1, 2, \ldots, s - 1,
\]

(72)

\[
\gamma_{k+1}' < \gamma_k', \quad k = 1, 2, \ldots, s - 2.
\]

(73)

**Proof.** In the multiple singular value case, as we have shown in section 3, algorithm 1 can only be run to step $s$ without breakdown. From (41), we augment $P_{s+1}$ and $Q_s$ to the $m \times m$ and $n \times n$ orthogonal matrices $P = (P_{s+1}, \hat{P})$ and $Q = (Q_s, \hat{Q})$, respectively. Then from (41) we obtain

\[
P^T AQ = P^T A' Q = \begin{pmatrix} B_k & 0 \\ 0 & 0 \end{pmatrix},
\]

from which it follows that

\[
\gamma_k' = \|A' - P_{k+1} B_k Q_k^T\| = \|P^T (A' - P_{k+1} B_k Q_k^T) Q\| = \|G_k'\|,
\]

where $G_k'$ is the right bottom $(s - k + 1) \times (s - k)$ matrix of $B_k$. Then the remaining proof is exactly the same as that of the theorem 5.1 in [34]. \(\square\)

**Remark 6.1.** The strict decreasing property (73) of $\gamma_k'$ and the lower bounds for $\gamma_k'$ in (71) and (72) hold unconditionally, independently of the degree of ill-posedness of problem (23).

**Remark 6.2.** It is impractical to compute $\gamma_k'$ for $A$ large. Fortunately, (71) and (72) indicates that the sum $\alpha_{k+1} + \beta_{k+2} \leq \sqrt{2} \gamma_k'$ decays as fast as $\gamma_k'$. Therefore, we can reliably judge the decay rates of $\gamma_k'$ during computation with little extra cost.

**Remark 6.3.** For the severely and moderately ill-posed problems with suitable $\rho > 1$ and $\alpha > 1$, (71) and (72) show that $\alpha_{k+1} + \beta_{k+2}$ decays as fast as $\sigma_{k+1}$ for $k \leq k_0$. For mildly ill-posed problems, since $\eta_k$ becomes bigger than one considerably as $k$ increases, $\alpha_{k+1} + \beta_{k+2}$ cannot generally decay as fast as $\sigma_{k+1}$.

7. Best, near best and general rank $k$ approximations to $A$ and their implications on LSQR and some other Krylov solvers

In this section, we consider some important issues on best, near best and general rank $k$ approximations to $A$ when all the singular values of $A$ are simple, i.e., the multiplicities $c_i = 1, i = 1, 2, \ldots, s$ and $s = n$. The issues to be addressed has received no attention in [33, 34].
and the literature, but may be valuable in a variety of applications of low rank approximations. As far as LSQR is concerned in the context of discrete ill-posed problems, based on the previous results and analysis, if $A$ has at least one multiple singular value, i.e., some $c_i > 1$, then we speak of the corresponding rank $k$ approximations to $A'$. Therefore, for the uniqueness, without loss of generality, in this section we assume that $A' = A, \Sigma' = \Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n), U = (u_1, u_2, \ldots, u_n)$ and $V = (v_1, v_2, \ldots, v_n)$ in (16), and the compact SVD of $A$ is $A = U \Sigma V^T$.

We denote by

$$\gamma_k = \|A - P_{k+1}B_kQ_k^T\|, \quad k = 1, 2, \ldots, n - 1$$

(74)

the accuracy of the rank $k$ approximation $P_{k+1}B_kQ_k^T$ to $A$.

We first investigate general best or near best rank $k$ approximations to $A$ with $\sigma_k = \zeta k^{-\alpha}$ and $\alpha > 0$. We will show that, for each of such rank $k$ approximations, its smallest nonzero singular value may be smaller than $\sigma_{k+1}$ for $\alpha \leq 1$, that is, its nonzero singular values may not approximate the $k$ large singular values of $A$ in natural order, but it is guaranteed to be bigger than $\sigma_{k+1}$ for suitable $\alpha > 1$. The implication is that a general best or near best rank $k$ approximation to $A$ may have very small nonzero singular values and thus may not be a suitable replacement for $A$ for $\alpha \leq 1$. We then consider the properties of the Ritz values $\theta_i^{(k)}$, $i = 1, 2, \ldots, k$ and derive some interesting properties on them when $P_{k+1}B_kQ_k^T$ is or is not a near best rank $k$ approximation to $A$ for the ill-posed problems with $0 < \alpha \leq 1$, which include mildly ill-posed ones. Finally, we elaborate how to apply these properties to several other Krylov solvers used to solve ill-posed problems.

First of all, we mention an intrinsic fact that the best rank $k$ approximations to $A$ with respect to the two-norm are not unique. In fact, besides $A_k = U_k \Sigma_k V_k^T$ with $U_k = (u_1, u_2, \ldots, u_k)$, $V_k = (v_1, v_2, \ldots, v_k)$ and $\Sigma_k = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_k)$, there are other infinitely many best rank $k$ approximations to $A$. This is certainly also true for near best rank $k$ approximations to $A$, as we see below.

Let $C_k$ be a best or near best rank $k$ approximation to $A$ with $\|A - C_k\| = (1 + \epsilon)\sigma_{k+1}$ with any $\epsilon \geq 0$ satisfying $(1 + \epsilon)\sigma_{k+1} < \frac{\sigma_k}{\epsilon + \sigma_k}$, that is, $(1 + \epsilon)\sigma_{k+1}$ is between $\sigma_{k+1}$ and $\sigma_k$ and closer to $\sigma_{k+1}$ (note: $\epsilon = 0$ corresponds to a best rank $k$ approximation $C_k$). Then we have

$$1 + 2\epsilon < \frac{\sigma_k}{\sigma_{k+1}}.$$  

(75)

It is remarkable to note that $C_k$ is not unique for any given $\epsilon \geq 0$ satisfying (75). For example, among others, it is easy to verify that all the matrices

$$C_k = A_k(\theta, j) = A_k - \sigma_{k+1} U_k \text{diag}(\theta(1 + \epsilon), \ldots, \theta(1 + \epsilon), \theta(1 + \epsilon), \ldots, \theta(1 + \epsilon)) V_k^T$$  

(76)

with any $\theta \in [0, 1]$ and $1 \leq j \leq k - 1$ form a family of best or near best rank $k$ approximations to $A$ that satisfy $\|A - C_k\| = (1 + \epsilon)\sigma_{k+1}$. Meanwhile, it is easily seen that the smallest nonzero singular value of $C_k$ is $\sigma_k - \theta(1 + \epsilon)\sigma_{k+1}$.

**Theorem 7.1.** Let $C_k$ be the best or near best approximations to $A$ defined as (76). Then for $0 < \alpha \leq 1$, if $\theta$ is sufficiently close to one and $k > 1$, it holds that

$$\sigma_k - \theta(1 + \epsilon)\sigma_{k+1} < \sigma_{k+1}.$$  

(77)
that is, the smallest nonzero singular value \( \sigma_k - \theta(1 + \epsilon)\sigma_{k+1} \) of \( C_k \) does not lie between \( \sigma_{k+1} \) and \( \sigma_k \); if \( \theta \) is sufficiently close to zero, then \( \sigma_k - \theta(1 + \epsilon)\sigma_{k+1} \) lies in \( \sigma_{k+1} \) and \( \sigma_k \):

\[
\sigma_{k+1} < \sigma_k - \theta(1 + \epsilon)\sigma_{k+1} < \sigma_k.
\] (78)

If \( \alpha > 1 \) sufficiently, (78) holds for \( k > 1 \) and any \( \theta \in [0, 1] \).

**Proof.** Since \( \sigma_k = \zeta_k^{-\alpha} \) and \( \left( \frac{k+1}{k} \right)^{\alpha} < 2 \) for any \( k > 1 \) and \( 0 < \alpha < 1 \), we obtain

\[
\sigma_k - \theta(1 + \epsilon)\sigma_{k+1} = \sigma_{k+1} \left( \left( \frac{k+1}{k} \right)^{\alpha} - \theta(1 + \epsilon) \right) < \sigma_{k+1}
\] (79)

for \( \theta \) sufficiently close to one. This shows that \( \sigma_k - \theta(1 + \epsilon)\sigma_{k+1} \) does not lie between \( \sigma_{k+1} \) and \( \sigma_k \) and does not interlace them for \( k > 1 \). In this case, for a given \( \alpha \leq 1 \), the bigger \( k \) is, the smaller \( \left( \frac{k+1}{k} \right)^{\alpha} - \theta(1 + \epsilon) \) is, and the further is \( \sigma_k - \theta(1 + \epsilon)\sigma_{k+1} \) away from \( \sigma_{k+1} \). On the other hand, for \( \theta \) sufficiently small we have

\[
\left( \frac{k+1}{k} \right)^{\alpha} - \theta(1 + \epsilon) > 1,
\] (80)

that is, \( \sigma_k - \theta(1 + \epsilon)\sigma_{k+1} \) interlaces \( \sigma_{k+1} \) and \( \sigma_k \) for \( \theta \) sufficiently small.

For \( A \) with \( \sigma_k = \zeta_k^{-\alpha} \) and \( \alpha > 1 \) and \( k = 1, 2, \ldots, n - 1 \), the requirement (80) is met for any \( \theta \in [0, 1] \) and suitable \( \alpha > 1 \), leading to \( \sigma_k - \theta(1 + \epsilon)\sigma_{k+1} > \sigma_{k+1} \). This means that the smallest nonzero singular value \( \sigma_k - \theta(1 + \epsilon)\sigma_{k+1} \) of the best or near best rank approximation \( C_k \) lies between \( \sigma_{k+1} \) and \( \sigma_k \) for suitable \( \alpha > 1 \). 

We should be aware that (77) is established by assuming the worst case that, over all best or near best rank \( k \) approximations \( C_k \) of form (76), the minimum \( \sigma_k - (1 + \epsilon)\sigma_{k+1} \) of the smallest nonzero singular values of the \( C_k \) is almost or exactly attained, i.e., \( \theta \approx 1 \) or \( \theta = 1 \).

We now prove that the minimum is indeed \( \sigma_k - (1 + \epsilon)\sigma_{k+1} \) over the set of all the near best rank \( k \) approximations \( C_k \), including the ones of form (76). Let \( \sigma_k(C_k) \) be the smallest nonzero singular value of \( C_k \). Then from \( \| A - C_k \| = (1 + \epsilon)\sigma_{k+1} \), by the standard perturbation theory we have

\[
|\sigma_k - \sigma_k(C_k)| \leq (1 + \epsilon)\sigma_{k+1}.
\]

Clearly, the minimum of all the \( \sigma_k(C_k) \) is attained if and only if the above equality holds and the left-hand side is positive, which means that this minimum is exactly \( \sigma_k - (1 + \epsilon)\sigma_{k+1} \). In contrast, (78) holds essentially in the best case that the maximum of the smallest singular values \( \sigma_k - \theta(1 + \epsilon)\sigma_{k+1} \) of \( C_k \) defined by (76) is almost or exactly taken, i.e., \( \theta \approx 0 \) or \( \theta = 0 \).

The above results indicate that, unlike for severely and moderately ill-posed problems with suitable \( \rho > 1 \) and \( \alpha > 1 \), a best or near best rank \( k \) approximation to \( A \) does not mean that its nonzero singular values approximate the large singular values of \( A \) in natural order and such a rank \( k \) approximation matrix may have nonzero singular values that are (much) smaller than \( \sigma_{k+1} \). As a consequence, replacing \( A \) by its excellent rank \( k \) approximation may be at risk in a variety of applications since such replacement may be unable to remove the effects of possible nonzero singular values much smaller than \( \sigma_{k+1} \).

As far as LSQR is concerned, notice from [34] that condition (69) for the interlacing property (70) is derived by assuming the worst case that \( \sigma_k - \theta_k^{(k)} = \gamma_k \leq \sqrt{1 + \eta_k^2} \sigma_{k+1} \), that is, \( \theta_k^{(k)} \) is supposed to be the smallest possible nonzero one among all the \( \sigma_k(C_k) \), where \( C_k \) belongs to the set of near best \( k \) approximations that satisfy \( \| A - C_k \| = \gamma_k \leq \sqrt{1 + \eta_k^2} \sigma_{k+1} \).
Even so, a near best rank $k$ approximation $P_{k+1}B_kQ_k^T$ can guarantee the approximations of $\theta_j^{(k)}$, $i = 1, 2, \ldots, k$ to the large singular values $\sigma_i$ in natural order for suitable $\alpha > 1$. This is in accordance with theorems 5.2 and 5.3 though the sizes of $\alpha > 1$ for them are different.

For mildly ill-posed problems, Theorem 7.1 and the above analysis indicate that the $k$ Ritz values $\theta_j^{(k)}$ may or may not approximate the large singular values $\sigma_j$ of $A$ in natural order even when $P_{k+1}B_kQ_k^T$ is a near best rank $k$ approximation to $A$.

Unfortunately, as we have elaborated and numerically confirmed in [34], for mildly ill-posed problems, $P_{k+1}B_kQ_k^T$ may be a near best rank $k$ approximation to $A$ only for $k$ very small and it is not any more soon as $k$ increases. The following results are more general and cover all ill-posed problems with $0 < \alpha \leq 1$, which include mildly ill-posed ones. We will seek the maximum possible number of the Ritz values smaller than $\sigma_{k+1}$ and get insight into how small they can be.

**Theorem 7.2.** For $\sigma_i = \zeta j^{-\alpha}, i = 1, 2, \ldots, n$ with $0 < \alpha \leq 1$, suppose $\gamma_k \in [\sigma_{j+1}, \sigma_j]$ for some $j \leq k$. Then

(a) if $\gamma_k$ is closer to $\sigma_{j+1}$ than to $\sigma_j$ and $j(j + 1) \geq k$, there are at most $k - j + 1$ Ritz values $\theta_j^{(k)}, \theta_{j+1}^{(k)}, \ldots, \theta_k^{(k)}$ smaller than $\sigma_{k+1}$;

(b) if $j \geq 2$, $\gamma_k$ is closer to $\sigma_{j+1}$ than to $\sigma_j$, and $j(j + 1) > k$, there are at most $k - j + 2$ Ritz values $\theta_j^{(k)}, \theta_{j+1}^{(k)}, \ldots, \theta_k^{(k)}$ smaller than $\sigma_{k+1}$;

(c) if $j = 1$, $\gamma_k$ is closer to $\sigma_1$ than to $\sigma_2$, all the Ritz values $\theta_i^{(k)}$, $i = 1, 2, \ldots, k$ are possibly smaller than $\sigma_{k+1}$.

**Proof.** Since $\sigma_j = \zeta j^{-\alpha}$, we have

$$
\frac{\alpha}{j} \sigma_{j+1} = \frac{\alpha}{j} j^{-\alpha} \zeta j^{-\alpha} \sigma_{j+1} = \frac{\alpha}{j} j^{-\alpha} \zeta^2 j^{-\alpha} (j + 1)^{-\alpha}
= \frac{\alpha}{j} j^{-\alpha} (\sigma_{j+1}) = \frac{\alpha}{j} \sigma_{j+1}.
$$

(81)

Define the function $f(x) = (1 + x)^{\alpha}$ for $x > 0$ and $0 < \alpha \leq 1$. Then its $\ell$th derivative

$$
\frac{d^\ell}{dx^\ell} f(x) = \alpha (\alpha - 1) \cdots (\alpha - \ell + 1) (1 + x)^{(\alpha - 1)(\alpha - 2) \cdots (\alpha - \ell)}
$$

is always negative for $\ell \geq 2$. Therefore, taking the first three terms of the Taylor expansion of $f(\zeta) = (1 + \zeta)^{\alpha}$ and exploiting (81), we obtain

$$
\sigma_j - \sigma_{j+1} = \sigma_{j+1} \left( \left( \frac{j + 1}{j} \right)^{\alpha} - 1 \right) = \sigma_{j+1} \left( 1 + \frac{\alpha}{j} \frac{(1 - \alpha)\alpha}{2f} - 1 \right)
= \frac{\alpha}{j} \sigma_{j+1} \left( 1 - \frac{(1 - \alpha)\alpha}{2j} \right)
= \frac{\alpha}{j} \sigma_{j+1} \left( 1 - \frac{(1 - \alpha)\alpha}{2j} \right).
$$

(82)

In the case that $\gamma_k$ lies in $[\sigma_{j+1}, \sigma_j]$ and is closer to $\sigma_{j+1}$ than to $\sigma_j$, for $1 \leq j < k$, by taking $i = j$ in (68), we get $\sigma_j - \theta_j^{(k)} \leq \gamma_k$. Therefore, by the assumption on $\gamma_k$, from (82) we obtain
the lower bounds for $\theta_j^{(k)}$:

$$\theta_j^{(k)} \geq \sigma_j - \gamma_k \geq \frac{\sigma_j - \sigma_{j+1}}{2} \geq \frac{\alpha}{2j^{1-\alpha}} \sigma_{j(j+1)} \left( 1 - \frac{(1 - \alpha)}{2j} \right), \quad (83)$$

Since each lower bound in (83) cannot be improved, $\theta_j^{(k)}$ is always likely to (approximately) attain the second lower bound. Suppose it is the case, and note that $\frac{\alpha}{2j^{1-\alpha}} < 1$ decreases with $j$ for a given $\alpha \in (0, 1)$ and equals one for $\alpha = 1$. We then obtain

$$\theta_j^{(k)} \approx \frac{\alpha}{2j^{1-\alpha}} \sigma_{j(j+1)} \left( 1 - \frac{(1 - \alpha)}{2j} \right) \leq \frac{\alpha}{2j^{1-\alpha}} \sigma_{j(j+1)} \leq \frac{1}{2} \sigma_{j(j+1)} < \sigma_{j(j+1)},$$

which is smaller than $\sigma_{k+1}$ when $j(j+1) > k$.

Moreover, whenever $\theta_j^{(k)} < \sigma_{k+1}$, by the labeling rule, there are $k - j + 1$ Ritz values $\theta_j^{(k)}, \theta_{j+1}^{(k)}, \ldots, \theta_k^{(k)}$ smaller than $\sigma_{k+1}$.

We next analyze the case that $\gamma_k$ lies in $[\sigma_{j+1}, \sigma_j]$ and is closer to $\sigma_1$ than to $\sigma_{j+1}$ for $j \geq 2$. Taking $i = j - 1$ in (68), we have $\sigma_{j-1} - \theta_{j-1}^{(k)} \leq \gamma_k$, which shows that

$$\theta_{j-1}^{(k)} \geq \sigma_{j-1} - \gamma_k.$$ 

For $\sigma_j = \zeta^j$ with $\alpha > 0$, it is easy to justify that

$$\sigma_{j-1} - \sigma_j > \sigma_j - \sigma_{j+1}.$$ 

Therefore, from (82) we obtain

$$\theta_{j-1}^{(k)} \geq \sigma_{j-1} - \gamma_k \geq \sigma_{j-1} - \sigma_j > \sigma_j - \sigma_{j+1} \geq \frac{\alpha}{j^{1-\alpha}} \sigma_{j(j+1)} \left( 1 - \frac{(1 - \alpha)}{2j} \right).$$

Analogously, when the above lower bound is (approximately) attainable, for $j \geq 2$ we have

$$\theta_{j-1}^{(k)} \approx \frac{\alpha}{j^{1-\alpha}} \sigma_{j(j+1)} \left( 1 - \frac{(1 - \alpha)}{2j} \right) \leq \frac{\alpha}{j^{1-\alpha}} \sigma_{j(j+1)} \leq \sigma_{j(j+1)},$$

which is smaller than $\sigma_{k+1}$ when $j(j+1) > k$.

Whenever $\theta_{j-1}^{(k)} < \sigma_{k+1}$, by the labeling rule, there are $k - j + 2$ Ritz values $\theta_{j-1}^{(k)}, \theta_{j}^{(k)}, \ldots, \theta_k^{(k)}$ smaller than $\sigma_{k+1}$.

The above analysis does not include the case that $j = 1$ and $\gamma_k$ is closer to $\sigma_1$ than to $\sigma_2$, which needs a special treatment. For this case, taking $i = 1$ in (68) yields $\sigma_1 - \theta_1^{(k)} \leq \gamma_k$, from which we obtain

$$\theta_1^{(k)} \geq \sigma_1 - \gamma_k.$$ 

Under the assumption, such lower bound can be arbitrarily small, which means that $\theta_1^{(k)}$ can be arbitrarily small so that it can be smaller than $\sigma_{k+1}$. The closer $\gamma_k$ is to $\sigma_1$, the more likely $\theta_1^{(k)} < \sigma_{k+1}$. As a consequence, it is possible that all the Ritz values $\theta_i^{(k)}, i = 1, 2, \ldots, k$ are smaller than $\sigma_{k+1}$. \hfill \Box

This theorem indicates that, whenever $j(j+1) > k$ substantially, $\theta_j^{(k)}$ or $\theta_{j-1}^{(k)} \approx \sigma_{j(j+1)}$ can be considerably smaller than $\sigma_{k+1}$. Furthermore, we see from (81) and the proof that for $j \geq 2$, the smaller $\alpha < 1$, the smaller $\frac{\alpha}{j^{1-\alpha}} \sigma_{j(j+1)}$ is than $\sigma_{j(j+1)}$, and, for a fixed $\alpha < 1$, the bigger $j$, the smaller $\frac{\alpha}{j^{1-\alpha}} \sigma_{j(j+1)}$ than $\sigma_{j(j+1)}$. Consequently, the smaller $\alpha < 1$, the more likely is $\theta_j^{(k)}$ or $\theta_{j-1}^{(k)}$.
smaller than \( \sigma_{k+1} \) when \( j(j+1) > k \). Even for \( j = k \), this theorem illustrates that a near best approximation \( P_{k+1} B_k Q_k^T \) does not guarantee that \( \theta_{i(k)}^j \), \( i = 1, 2, \ldots, k \) approximate the large singular values \( \sigma_i \) of \( A \) in natural order; in the worst case, we may have \( \theta_{i(k)}^k < \sigma_{k(k+1)} \).

More generally, if \( P_{k+1} B_k Q_k^T \) is replaced by any rank \( k \) approximation \( C_k \) to \( A \) and we still denote \( \gamma_k = |A - C_k| \) and by \( \theta_{i(k)}^k \) the \( k \) nonzero singular values of \( C_k \) by requiring that \( \theta_{i(k)}^k \leq \sigma_i \), \( i = 1, 2, \ldots, k \), then this theorem still holds. Therefore, for such \( C_k \) and \( 0 < \alpha \leq 1 \), the nonzero singular values of \( C_k \) do not necessarily approximate the large singular values of \( A \) in natural order, and some of them may be smaller than \( \sigma_{k+1} \).

MINRES and MR-II are Krylov solvers for (1) with \( A \) symmetric and have been shown to have regularizing effects [18, 21, 25, 31, 32, 39], but MR-II is preferable since the noisy \( b \) is excluded in the underlying subspace [31, 32]. For \( A \) nonsymmetric or multiplication with \( A^T \) difficult to compute, GMRES and RRGMRES are candidate methods, and the latter may be better [32]. We mention that the regularizing effects of GMRES and RRGMRES are highly problem dependent, and it appears that they require that the mixing of the left and right singular vectors of \( A \) be weak, that is, \( V^T U \) is close to a diagonal matrix; see, e.g., [32] and [25, p 126].

Similar to LSQR, all the above methods and CGME [4, 5, 10, 18, 19] generate their own rank \( k \) approximations to \( A \) at iteration \( k \). For each of these rank \( k \) approximation to \( A \), still denote by \( \theta_{i(k)}^j \), \( i = 1, 2, \ldots, k \) its nonzero singular values. Since the first inequality of (68) holds for all these methods. As a consequence, theorem 7.2 holds for all of them, and its proof carries over to these methods without any change.

However, we must point out that, for a given (1), the size and properties of \( \gamma_k \) in these methods differ greatly, so is the approximation behavior of \( \theta_{i(k)}^j \), \( i = 1, 2, \ldots, k \). For example, \( \gamma_k \) in CGME monotonically decreases strictly with respect to \( k \), and is unconditionally bigger than that in LSQR [35]. Though not explicitly presented in [31], using the analysis approach in [34, 35], we can easily prove that \( \gamma_k \) in MINRES or MR-II monotonically decreases with respect to \( k \). Such monotonic decreasing property of \( \gamma_k \) has turned out to be extremely important for a Krylov solver in the context of ill-posed problems since the rank \( k \) approximation is becoming an increasingly better replacement of \( A \) when \( \gamma_k \) decreases monotonically. If the Krylov solver does not have this property, it may not be a good regularization method for solving (1). Unfortunately, for a general nonsymmetric \( A \), it can be justified that the \( \gamma_k \) in GMRES and RRGMRES, mathematically, do not have such monotonic decreasing property, and can behave very irregularly as \( k \) increases. These mean that these two methods could not have regularizing effects and may not find any meaningful regularized solutions.

### 8. Numerical experiments

In this section, we present numerical experiments to justify and get insight into theorems 4.1, 4.2 and 5.3 and the behavior of the TSVD method when \( A \) has multiple singular values, theorems 5.2, 5.3, 6.1, 7.1 and 7.2 when \( A \) has only simple singular values. The extensive experiments in [33–35] have confirmed the other results as well as theorems 5.2, 5.3 and 6.1 when the singular values \( \sigma_i \) of \( A \) are all simple, and we will report more experiments to get more insight into these three theorems when the singular values of \( A \) are all simple.

To illustrate theorems 4.1, 4.2 and 5.3 and the TSVD method when \( A \) has multiple singular values, we test problems PRblurgauss, PRblurrotation and PRtomo from [15] where the matrices \( A \) have been found to have many multiple singular values, that is, many consecutive singular values are numerically equal within a small multiple of \( ||A|| \) times the machine precision. As for theorems 7.1 and 7.2, we use some random matrices regutm from [24] to generate the test problems, and the Matlab function \([A,U,V] = \text{regutm}(m,n,s)\) constructs a
Table 1. The description of test problems.

| Problem      | Description               | Ill-posedness | $m \times n$     |
|--------------|---------------------------|---------------|------------------|
| PRblurgauss  | Image deblurring          | Severe        | 10,000 $\times$ 10,000 |
| PRblurrotation| Image beblurring          | Mild          | 16,384 $\times$ 16,384 |
| PRtomo       | X-ray computerized tomography | Mild       | 25,380 $\times$ 10,000 |
| regutm       | Random ill-posed problem  | Mild or moderate | 10,000 $\times$ 10,000 |

random $m \times n$ matrix $A$ with $m \geq n$ in the normal distribution such that the eigenvectors $u_k$ and $v_k$ of $AA^T$ and $A^TA$ are oscillating:

$$ A = U \text{diag}(S)V^T, $$

where the number of sign changes in the columns $u_k$ and $v_k$ of $U$ and $V$ is exactly $k - 1$, $k = 1, 2, \ldots, n$, and the third argument $S$ specifies the singular values $\sigma_j$ of $A$. We will take $\sigma_k = k^{-\alpha}$ for several $\alpha > 0$ and construct mildly and moderately ill-posed problems. Table 1 lists the test problems and some details, where we set $\text{options.Blurlevel} = \text{"severe"}$ in PRblurgauss and PRblurrotation and the other parameters are defaults except the matrix orders.

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.

In our experiments, we generate a Gaussian white noise vector $e$ with zero mean and the relative noise level

$$ \varepsilon = \frac{\|e\|}{\|b_{\text{true}}\|}, $$

and add it to $b_{\text{true}}$ to form the noisy right-hand side $b$. We use the LSQR algorithm with the starting vector $b/\|b\|$ to solve problem (1). To simulate exact arithmetic, we use algorithm 1 with reorthogonalization to generate $B_k$ and numerically orthonormal $P_{k+1}$ and $Q_k$.

For PRblurgauss, generating a Gaussian noise with $\varepsilon = 0.1$, we add $e$ to $b_{\text{true}}$ and form a noisy $b$. In all the experiments, for our convenience, unlike what we do in sections 2–6, we denote the singular values of $A$ by $\sigma_i$, $i = 1, 2, \ldots, n$ without counting multiplicities and label them in descending order without counting multiplicities, i.e., $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$. This is a multiple singular value problem. For example, among the first 40 singular values, we have found that

$$\begin{align*}
\sigma_2 &= \sigma_3, \\
\sigma_5 &= \sigma_6, \\
\sigma_7 &= \sigma_8, \\
\sigma_{10} &= \sigma_{11}, \\
\sigma_{12} &= \sigma_{13}, \\
\sigma_{14} &= \sigma_{15}, \\
\sigma_{16} &= \sigma_{18}, \\
\sigma_{18} &= \sigma_{19},
\end{align*}$$

$$\begin{align*}
\sigma_{21} &= \sigma_{22}, \\
\sigma_{23} &= \cdots = \sigma_{26}, \\
\sigma_{27} &= \sigma_{28}, \\
\sigma_{29} &= \sigma_{30}, \\
\sigma_{32} &= \sigma_{33}, \\
\sigma_{34} &= \sigma_{35},
\end{align*}$$

$$\begin{align*}
\sigma_{36} &= \sigma_{37}, \\
\sigma_{38} &= \sigma_{39},
\end{align*}$$

as is visually seen from figure 1(d). Furthermore, we have found that the average decay rate of the distinct ones among the first 1500 singular values is approximately $\rho^{-1} = 0.9697$, i.e., $\rho = 1.0312$, which means that problem (23) is only slightly severely ill-posed. Therefore, from theorems 5.2 and 5.3, this problem does not satisfy the sufficient conditions that algorithm 1 generates near best approximations to $A'$ and the Ritz values $\theta_j^{(k)}$ approximate the first $k$ large singular values of $A'$ in natural order at all iterations $k \leq k^*$. As is depicted in figure 1(b), the
semi-convergence of the TSVD method for PRblurguass occurs at the optimal regularization parameter $c_1 + c_2 + \cdots + c_k = 276$, and we have verified that the number of distinct ones in the first 276 singular values of $A$ is 121, which is the optimal regularization parameter $k_0$ of the TSVD method for solving problem (23). Figure 1(a) indicates that LSQR computes its best regularized solution at $k^* = 13$, much smaller than $k_0 = 121$. But figures 1(a) and (b) clearly demonstrate that the two best possible regularized solutions obtained by LSQR and the TSVD method have essentially the same accuracy, showing that LSQR has the full regularization.

Note that $k^* < k_0$. Theorem 4.1 indicates that in this case the Ritz values $\theta_j^{(k)}$ must not converge to the first $k$ large singular values of $A'$, i.e., the first $k$ distinct singular values of $A$, in natural order for some $k < k^*$. This is indeed true, as can be seen from figure 1(c), which depicts the first 15 distinct singular values of $A$ and the $\theta_j^{(k)}$ at $k = k^* = 13$. More precisely, the first three $\theta_j^{(13)}$ approximate the first three distinct large singular values of $A$ and the fourth to the thirteenth ones fail to approximate the large distinct singular values of $A$ in natural order. These results justify not only theorem 4.1 but also theorems 4.2 and 5.3. Unfortunately, we are unable to numerically justify theorem 5.2 explicitly since $A'$ cannot be formed accurately in finite precision arithmetic by noticing that the singular triplets of $A$ corresponding to small singular values could not be computed accurately and they even have no accuracy at all when the singular values are at or below the level of $\|A\|\epsilon_{\text{mach}}$. Actually, $\sigma_{3200} \approx \|A\|\epsilon_{\text{mach}}$ already for this problem. Therefore, the standard Matlab code $\text{svd}$ may compute $(\sigma, u_i, v_i), i = 3200, \ldots, 10000$ with no accuracy. However, the non-computability of $A'$ with high accuracy does not obsess us and causes no essential difficulty. The reason is that the approximation accuracy of rank $k$ approximations to $A'$ is intimately related to the convergence behavior of Ritz values for
severely and moderately ill-posed problems: if the Ritz values \( \theta_j^{(k)} \) fail to approximate the \( k \) large distinct singular values of \( A \), then the corresponding rank \( k \) approximation is not a near best one, and vice versa, as theorems 5.2 and 5.3 imply. Therefore, we can deduce that \( P_{k+1}B_kQ_k^T \) is not a near best rank \( k \) approximation to \( A' \) for some \( k \leq k^* \) for PRblurgauss.

The behavior of the TSVD method deserves special attention in the multiple singular value case. Recall our comment paragraph on relations (8) and (9). We have observed from figure 1(d) that, before the occurrence of semi-convergence, the errors of TSVD regularized solutions decrease slowly at a multiple singular value when the TSVD method does not yet exploit the full right and left singular subspace associated with a \( c_k \) multiple singular value, that is, only \( c_{\tilde{k}} < c_k \) left and right singular vectors are included in the TSVD solutions, and the errors continue to essentially decrease after \( c_{\tilde{k}} = c_k \) and when a GSVD component of the next distinct singular value starts to emerge in a new TSVD solution.

For the mildly ill-posed problems PRblurrotation and PRTomo, theorems 4.2 and 5.3 have shown that algorithm 1 generally cannot generate near best rank \( k \) approximations to \( A' \), and the Ritz values \( \theta_j^{(k)} \) fail to converge to the first \( k \) singular values of \( A' \) in natural order at some \( k \leq k^* \), so that we must have \( k^* < k_0 \), where \( k_0 \) is the semi-convergence point of the TSVD method applied to problem (23), which corresponds to the semi-convergence point \( c_1 + c_2 + \cdots + c_{k_0} \) of the TSVD method applied to problem (1).

Numerical experiments confirm the above results, where we take the relative noise level \( \varepsilon = 0.01 \) and 0.1 for PRblurrotation and PRTomo, respectively; see figures 2 and 3, where similar remarks to PRblurgauss can be made and LSQR has exhibited its full regularization ability. For PRblurrotation, we have found that five pairs in its first twenty singular values are double multiple, which are \( \sigma_2 = \sigma_3, \sigma_7 = \sigma_8, \sigma_9 = \sigma_{10}, \sigma_{15} = \sigma_{16} \) and \( \sigma_{18} = \sigma_{19} \).
as can be visually seen from figure 2(d). A slight difference between figures 2(d) and 1(d) is that the phenomenon observed and commented above for PRblurgauss is not so apparent visually for PRblurrotation. The reason is that the distinct singular values of PRblurrotation decay much more slowly than the ones of PRblurgauss, a remarkable difference between severely and mildly ill-posed problems. Consequently, the TSVD method needs much bigger $k_0$ for a mildly ill-posed one than for a severely ill-posed one with the same level relative noise level, and, correspondingly, solutions errors decrease much more slowly, as is seen from figure 2(d).

We have justified that the distinct singular values of PRtomo decay more slowly than those of PRblurrotation. In figure 3 we do not depict a figure similar to figures 1(d) and 2(d) as we have found that the visuality of such figure is poorer for this problem than figure 2(d), though the actual data expose similar phenomena. Instead, we depict the first twenty large singular values of PRtomo in figure 3(d), among them, we have found that three pairs are multiple: $\sigma_2 = \sigma_3, \sigma_6 = \sigma_7$ and $\sigma_{15} = \sigma_{16}$. Actually, $A$ has many multiple singular values, and we do not give more details here. Remarkably, unlike the severely ill-posed PRblurgauss where the singular value decay much faster, the TSVD method for these two mildly ill-posed problems needs much bigger regularization parameter $k_0$ for (23) and thus $c_1 + c_2 + \ldots + c_0$, for (1), that is, the method uses many more SVD components to form the best regularized solutions, compared with the TSVD method for PRblurgauss, as we can see from figures 1(b)–3(b). Importantly, as we have seen from figures 2 and 3, the best possible regularized solutions by LSQR are at least as accurate as those by the TSVD method, showing that the LSQR has the full regularization for these two mildly ill-posed problems.
Finally, we use the test problem regutm to justify theorems 7.1 and 7.2. We take \( \sigma_k = k^{-\alpha} \), \( k = 1, 2, \ldots, n \) by taking \( m = n = 10000 \) and \( \alpha = 1, 0.6 \) and 0.3, respectively, which meet the assumptions of theorems 7.1 and 7.2. We construct the exact solution \( x_{\text{true}} = \text{ones}(n, 1) \) and then noise free right-hand side \( b_{\text{true}} = Ax_{\text{true}} \). Then we generate a Gaussian noise vector \( e \) with the relative noise level \( \epsilon = 10^{-3} \), and add it to \( b_{\text{true}} \) to form the noisy right-hand side \( b \). Here we are only concerned with the accuracy \( \gamma_k \) of the rank \( k \) approximations \( P_{k+1}B_kQ_k^T \) to \( A \) and the approximation behavior of the Ritz values \( \theta_j^{(k)} \), \( i = 1, 2, \ldots, k \).

Figures 4–6(a) draw the accuracy \( \gamma_k \) of rank \( k \) approximations \( P_{k+1}B_kQ_k^T \) and \( \sigma_{k+1} \), and figures 4–6(b) depict the locations of the \( k \) Ritz values \( \theta_j^{(k)} \) and the first \( k+1 \) large singular values \( \sigma_i \) of \( A \) for the three \( \alpha \)'s. Table 2 highlights these figures and lists some precise results, where the first column indicates the location of \( \gamma_k \) and to which singular value it is closer, and the second column ‘near best’ indicates whether or not \( P_{k+1}B_kQ_k^T \) is a near best rank \( k \) approximation to \( A \) in the sense of (46), the third column ‘\# < \sigma_{k+1}’ denotes the number of \( \theta_j^{(k)} < \sigma_{k+1} \), \( i = 1, 2, \ldots, k \), and the fourth column ‘\# attained’ denotes whether or not the number in the third column attains the maximum possible number of \( \theta_j^{(k)} < \sigma_{k+1} \), \( i = 1, 2, \ldots, k \), which is indicated in theorem 7.2.

Several comments are made in order on figures 4–6 and table 2. Firstly, for the test problem with \( \alpha = 1 \), we observe from figure 4(a) that \( P_{k+1}B_kQ_k^T \) is a near best rank \( k \) approximation to \( A \) for \( k = 1, 2, \ldots, 6 \) and afterwards it is not any longer. However, starting from \( k = 5 \) onwards, the \( \theta_j^{(k)} \) do not approximate the \( k \) large singular values \( \sigma_i \) of \( A \) in natural order, as is clearly displayed in figure 4(b). This indicates that the near best rank \( k \) approximations for \( k = 5, 6 \) cannot guarantee that the \( \theta_j^{(k)} \) approximate the \( \sigma_i \) in natural order, confirming our theory. Furthermore, it is seen from table 2 that in each of these two cases there is exactly one Ritz value \( \theta_j^{(k)} < \sigma_{k+1} \), which coincides with the maximum possible number estimated by theorem 7.2.

Secondly, by comparing (a) with (b) in figures 4–6 correspondingly, we observe that there is always at least one Ritz value \( \theta_j^{(k)} < \sigma_{k+1} \) whenever \( P_{k+1}B_kQ_k^T \) is not a near best rank \( k \) approximation to \( A \). We have described these features more clearly in table 2.

Thirdly, by inspecting figures 4–6 and table 2, we find that, for the same \( k \), the smaller \( \alpha \) is, the less accurate the rank \( k \) approximation, since for the same \( k \) it is clear that \( \gamma_k \) is further away from \( \sigma_{k+1} \), which can be seen from the interval in which \( \gamma_k \) lies. This justifies that it is harder to generate a good rank \( k \) approximation when the decay of the singular values becomes slower.
Particularly, the rank $k$ approximations are not near best for $\alpha = 0.6$ and 0.3 from iterations $k = 2$ and $k = 1$ upwards, respectively.

Fourthly, we observe from figures 4 and 5(b) that the smaller $\alpha$ is, the earlier the Ritz values $\theta_i^{(k)}$ fail to approximate the $\sigma_i$ in natural order. Precisely, we can see from the figures that such $k$’s are 5, 3 and 2 for $\alpha = 1$, 0.6 and 0.3, respectively. Generally, we deduce that the approximations in natural order fail sooner as the decay of the singular values is slower.

Fifthly, for each $\alpha$, we see from figures 4–6 and table 2 that as $k$ increases, the rank $k$ approximation generally becomes poorer and the number of $\theta_i^{(k)} < \sigma_{i+1}$ exhibits an increasing tendency.

Sixthly, for different $\alpha$, we observe from table 2 that for the same $k$ and the smaller $\alpha$, the number of $\theta_i^{(k)} < \sigma_{i+1}$, $i = 1, 2, \ldots, k$ is at least nondecreasing and often increases.

Seventhly, for each $\alpha$ and given maximum $k = 10$ there is always at least one iteration $j \leq k$ at which the number of $\theta_j^{(k)} < \sigma_{j+1}$ is exactly equal to its possible maximum; see the fourth column of table 2.

Next, we report the results on $\text{regutm}$ of $m = n = 10000$ with $\sigma_k = k^{-0.3}$, i.e., $\alpha = 2$, $x_{\text{true}} = \text{ones}(n, 1)$ and the relative noise level $\varepsilon = 10^{-3}$. This is a moderately ill-posed problem.
Figures 7(a) and (b) depict the accuracy interlace the first $\alpha > 0$ with the second part of theorem 7.1, which requires that $\alpha > 1$ sufficiently for a given not small $k$. They also confirm the second part of theorem 7.1, which requires that $\alpha > 1$ sufficiently for a given not small $k$, while $\alpha = 2$ cannot meet this requirement for $k > 7$.

Table 2. The accuracy $\gamma_k$ of rank $k$ approximations and the approximation behavior of the Ritz values $\theta_i^{(k)}$, $i = 1, 2, \ldots, k$.

| $\sigma_k = k^{-0.6}$, $k = 1, 2, \ldots, n$ | Near best $\# < \sigma_{k+1}$ $\#$ attained |
|---------------------------------------------|---------------------------------------------|
| $\gamma_5 \in (\sigma_6, \sigma_5)$ closer to $\sigma_6$ | Yes | 1 | Yes |
| $\gamma_6 \in (\sigma_7, \sigma_6)$ closer to $\sigma_7$ | Yes | 1 | Yes |
| $\gamma_7 \in (\sigma_8, \sigma_7)$ closer to $\sigma_7$ | No | 1 | No |
| $\gamma_8 \in (\sigma_9, \sigma_8)$ closer to $\sigma_9$ | No | 1 | No |
| $\gamma_9 \in (\sigma_{10}, \sigma_8)$ closer to $\sigma_{10}$ | No | 2 | No |

| $\sigma_k = k^{-0.3}$, $k = 1, 2, \ldots, n$ | Near best $\# < \sigma_{k+1}$ $\#$ attained |
|---------------------------------------------|---------------------------------------------|
| $\gamma_3 \in (\sigma_4, \sigma_3)$ closer to $\sigma_3$ | No | 1 | No |
| $\gamma_4 \in (\sigma_4, \sigma_3)$ closer to $\sigma_4$ | No | 1 | No |
| $\gamma_5 \in (\sigma_6, \sigma_5)$ closer to $\sigma_5$ | No | 1 | No |
| $\gamma_6 \in (\sigma_7, \sigma_6)$ closer to $\sigma_7$ | No | 2 | Yes |
| $\gamma_7 \in (\sigma_8, \sigma_7)$ closer to $\sigma_8$ | No | 2 | No |
| $\gamma_8 \in (\sigma_9, \sigma_8)$ closer to $\sigma_9$ | No | 2 | No |
| $\gamma_9 \in (\sigma_{10}, \sigma_9)$ closer to $\sigma_{10}$ | No | 2 | No |

with $\alpha > 1$ fairly. We aim to justify theorems 5.2 and 5.3 and the second part of theorem 7.1. Clearly, we observe from the figure that $P_{k+1}B_kQ_k^T$ is a near best rank $k$ approximation to $A$ until $k = 7$ and afterwards it is not any longer. Correspondingly, the Ritz values $\theta_i^{(k)}$ interlace the first $k + 1$ large singular values $\sigma_i$ until the same $k$. Afterwards, such interlacing property is lost, and the Ritz values do not approximate the singular values in natural order any more. These justify theorems 5.2 and 5.3, in which, for a fixed $\alpha > 1$, the sufficient conditions (67) and (69) fail to meet when $k$ increases up to some point, since the left-hand sides strictly increase and the right-hand sides strictly decrease with $k$ for the fixed $\alpha$. They also confirm the second part of theorem 7.1, which requires that $\alpha > 1$ sufficiently for a given not small $k$, while $\alpha = 2$ cannot meet this requirement for $k > 7$. 34
Figure 7. (a): The accuracy $\gamma_k$ of rank $k$ approximations and the singular values $\sigma_k = k^{-2}$; (b) the $k$ Ritz values $\theta_i^{(k)}$ and the first $k + 1$ large singular values $\sigma_i$.

Figure 8. $\gamma_k$ versus $\alpha_{k+1} + \beta_{k+2}$ for regutm of $m = n = 10000$ with $\alpha = 2, 1, 0.6$ and 0.3.

By comparing figure 7 with figures 4–6, we mention that $k = 7$ is considerably bigger than those for $\alpha = 1, 0.6$ and 0.3, after which $P_{k+1}B_kQ_k^T$ is not a near best rank $k$ approximation and the Ritz values fail to approximate the singular values in natural order. This again confirms that, for the same $k$, the rank $k$ approximation $P_{k+1}B_kQ_k^T$ is more accurate and the Ritz values are more likely to approximate the singular values in natural order for a bigger $\alpha$. 

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Finally, we justify theorem 6.1 and the first two remarks followed. Figure 8 depicts $\gamma_k$ versus $\alpha_{k+1} + \beta_{k+2}$ for regutm with $\alpha = 2, 1, 0.6$ and 0.3. Clearly, we see from the figure that $\alpha_{k+1} + \beta_{k+2}$ decays exactly as fast as $\gamma_k$. Therefore, independent of the degree of ill-posedness, we can reliably judge the decreasing property and tendency of the practically uncomputable accuracy $\gamma_k$ by the available $\alpha_{k+1} + \beta_{k+2}$ with little cost. In addition, it is clearly seen from the figure that $\gamma_k$ decays faster for a bigger $\alpha$ than for a smaller $\alpha$.

9. Conclusions

For the large-scale ill-posed problem (1), LSQR is a most commonly used Krylov solver for a general purpose. It has general regularizing effects and exhibits semi-convergence. If LSQR has already found best possible two-norm filtering regularized solutions, then it has the full regularization. In this case, we simply stop it after a few iterations of semi-convergence, and complicated hybrid variants are not needed. The semi-convergence point of LSQR, in principle, can be determined by a suitable parameter-choice method, such as the L-curve criterion and the discrepancy principle [23, 25].

In the simple singular value case, the author in [33, 34] has proved that, for the severely and moderately ill-posed problems with suitable $\rho > 1$ and $\alpha > 1$, the Ritz values $\theta_i^{\alpha}$ approximate the large singular values of $A$ in natural order until the semi-convergence, so that LSQR has the full regularization. On the other hand, however, if $\alpha > 1$ but close to one, the approximation in this order cannot be ensured; if $\alpha \leq 1$, such approximation property may hold only for $k$ very small. In this paper, we have nontrivially extended the results in [33, 34] to the multiple singular value case, and drawn the same conclusions. We have made numerical experiments on a few real-world problems to justify our regularization results on LSQR and the special behavior of the TSVD method in the multiple singular value case.

As a major contribution, we have made an in-depth analysis on best, near best and general rank $k$ approximations to $A$ for more general ill-posed problems with $\alpha > 0$, which include mildly ill-posed problems, and derived some insightful properties of the Ritz values $\theta_i^{\alpha}$, $i = 1, 2, \ldots, k$. Our results have shown that general best or near best rank $k$ approximations do not guarantee that $\theta_i^{\alpha}$, $i = 1, 2, \ldots, k$ approximate large singular values of $A$ in natural order for $0 < \alpha \leq 1$. We have proved that, for the same $k$, the smaller $\alpha$ is, the less accurate the rank $k$ approximation is, and the more Ritz values smaller than $\sigma_{k+1}$. Numerical experiments have confirmed the theoretical results. These results apply to the other Krylov solvers CGME, MINRES, MR-II, GMRES and RRGMRES as well.

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