APPROXIMATION ACCURACY OF THE KRYLOV SUBSPACES FOR LINEAR DISCRETE ILL-POSED PROBLEMS

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Abstract. For the large-scale linear discrete ill-posed problem \( \min_{x \in \mathbb{R}^n} \|Ax - b\| \) or \( Ax = b \) with \( b \) contaminated by white noise, the Lanczos bidiagonalization based Krylov solver LSQR and its mathematically equivalent CGLS, the Conjugate Gradient (CG) method implicitly applied to \( A^T Ax = A^T b \), are most commonly used, and CGME, the CG method applied to \( \min \| AA^T y - b \| \) or \( AA^T y = b \) with \( x = A^T y \), and LSMR, which is equivalent to the minimal residual (MINRES) method applied to \( A^T Ax = A^T b \), have also been choices. These methods have intrinsic regularizing effects, where the iteration number \( k \) plays the role of the regularization parameter. However, there has been no definitive answer to the long-standing fundamental question: can LSQR and CGLS find best possible regularized solutions? The same question is for CGME and LSMR too. At iteration \( k \), these four methods compute iterates from the same \( k \)-dimensional Krylov subspace when starting vectors are chosen properly. A first and fundamental step towards to answering the above question is to accurately estimate the accuracy of the underlying \( k \)-dimensional Krylov subspace approximating the \( k \)-dimensional dominant right singular subspace of \( A \). Assuming that the singular values of \( A \) are simple, we present a general \( \sin \Theta \) theorem for the 2-norm distances between the two subspaces, derive accurate estimates on them for severely, moderately and mildly ill-posed problems, and establish some relationships between the smallest Ritz values and these distances. Numerical experiments justify our estimates and theory.

Key words. Discrete ill-posed, full regularization, partial regularization, TSVD solution, semi-convergence, Lanczos bidiagonalization, LSQR, Krylov subspace, approximation accuracy

AMS subject classifications. 65F22, 15A18, 65F10, 65F20, 65R32, 65J20, 65R30

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

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

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

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

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 \([17, 33, 36, 53, 59]\). 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, 16, 17, 36, 44, 49, 50, 53, 59, 60, 87]. The theory and numerical treatments of \((1.2)\) can be found in [53, 54]. The right-hand side \( b = b_{\text{true}} + e \) is noisy and assumed to be contaminated by a white noise.

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

For a white noise $e$, we assume that $b_{\text{true}}$ satisfies the discrete Picard condition $\|A^T b_{\text{true}}\| \leq C$ with some constant $C$ for $n$ arbitrarily large [1, 20, 30, 31, 33, 36, 50]. It is a discrete analog of the Picard condition in the Hilbert space setting; see, e.g., [30], [33, p.9], [36, p.12] and [50, p.63]. Without loss of generality, assume that $Ax = b$ is consistent; otherwise, we replace $b$ by its orthogonal projection onto the range of $A$. Then the two dominating regularization approaches are to solve the following two equivalent problems:

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

with $\tau > 1$ slightly and general-form Tikhonov regularization

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

with $\lambda > 0$ the regularization parameter [33, 36, 70, 79, 80], where $L$ is a regularization matrix, and its suitable choice is based on a-priori information on $x_{\text{true}}$. Typically, $L$ is either the identity matrix $I$ or the scaled discrete approximation of a first or second order derivative operator. If $L = I$, (1.4) is standard-form Tikhonov regularization.

The case $L = I$ is of most common interests and our concern in this paper. From now on, we always assume $L = I$, for which the solutions to (1.1), (1.3) and (1.4) can be fully analyzed by the singular value decomposition (SVD) of $A$. Let

\[
A = U \left( \begin{array}{c} \Sigma \\ 0 \end{array} \right) V^T
\]

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

\[
x_{\text{naive}} = \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i} v_i = \sum_{i=1}^{n} \frac{u_i^T b_{\text{true}}}{\sigma_i} v_i + \sum_{i=1}^{n} \frac{u_i^T e}{\sigma_i} v_i = x_{\text{true}} + \sum_{i=1}^{n} \frac{u_i^T e}{\sigma_i} v_i
\]

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

The discrete Picard condition means that, on average, the Fourier coefficients $|u_i^T b_{\text{true}}|$ decay faster than $\sigma_i$ and enables regularization to compute useful approximations to $x_{\text{true}}$, which results in the following popular model that is used throughout Hansen’s books [33, 36] and the references therein as well as the current paper:

\[
|u_i^T b_{\text{true}}| = \sigma_i^{1+\beta}, \quad \beta > 0, \ i = 1, 2, \ldots, n,
\]

where $\beta$ is a model parameter that controls the decay rates of $|u_i^T b_{\text{true}}|$. The white noise $e$ has a number of attractive properties which play a critical role in the regularization analysis: its covariance matrix is $\eta^2 I$, the expected values $\mathcal{E}(\|e\|^2) = m\eta^2$ and $\mathcal{E}(|u_i^T e|) = \eta, \ i = 1, 2, \ldots, n$, so that $\|e\| \approx \sqrt{m}\eta$ and $|u_i^T e| \approx \sigma_i^{1/2} |e|$. 

\( \eta, i = 1, 2, \ldots, n; \) see, e.g., [33, p.70-1] and [36, p.41-2]. The noise \( e \) thus affects \( u_i^T b, i = 1, 2, \ldots, n, \) more or less equally. With (1.7), relation (1.6) shows that for large singular values the signal terms \( |u_i^T e|/\sigma_i \) are dominant relative to the noise terms \( |u_i^T b_{\text{true}}|/\sigma_i \), that is, the \( \sigma_i^3 \) are considerably larger than the \( \eta/\sigma_i \). Once \( |u_i^T b_{\text{true}}| \approx |u_i^T e| \) for small singular values, the noise \( e \) dominates \( |u_i^T b| \), and the terms \( u_i^T b_{\text{true}} \approx u_i^T e \) overwhelm \( x_{\text{true}} \) and thus must be filtered out. The transition or cutting-off point \( k_0 \) is such that

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

see [36, p.42, 98] and a similar description [33, p.70-1]. In this sense, the \( \sigma_k \) are divided into the \( k_0 \) large ones and the \( n - k_0 \) small ones.

The truncated SVD (TSVD) method [30, 33, 36] is a reliable method for solving (1.3), and it deals with a sequence of problems

\[
\min \| x \| \quad \text{subject to} \quad \| A_k x - b \| = \min
\]

starting with \( k = 1 \) onwards, where \( A_k = U_k \Sigma_k V_k^T \) is the best rank \( k \) approximation to \( A \) with respect to the 2-norm with \( U_k = (u_1, \ldots, u_k), V_k = (v_1, \ldots, v_k) \) and \( \Sigma_k = \text{diag}(\sigma_1, \ldots, \sigma_k) \); it holds that \( \| A - A_k \| = \sigma_{k+1} \) [8, p.12]. The solution to (1.9) is \( x_{\text{tsvd}} = A_k^T b \), called the TSVD regularized solution, which is the minimum 2-norm solution to

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

that replaces \( A \) by \( A_k \) in (1.1).

Based on the above properties of the white noise \( e \), it is known from [33, p.70-1] and [36, p.71, 86, 89] that the TSVD solutions

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

and \( x_{\text{tsvd}} \) is the best TSVD regularized solution to (1.1), i.e., \( \| x_{\text{true}} - x_{\text{tsvd}} \| = \min_{k=1,2,\ldots,n} \| x_{\text{true}} - x_{\text{tsvd}} \| \); \( x_{\text{tsvd}} \) balances the regularization and perturbation errors optimally, and \( \| A_k x_{\text{tsvd}} - b \| \approx \| e \| \) stabilizes for \( k \) not close to \( n \) after \( k > k_0 \). The index \( k \) plays the role of the regularization parameter.

Tikhonov regularization (1.4) with \( L = I \) is a filtered SVD method. For each \( \lambda \), the solution \( x_\lambda \) satisfies \( (A^T A + \lambda^2 I)x_\lambda = A^T b \), which replaces the ill-conditioned \( A^T A \) in normal equation of (1.1) by \( A^T A + \lambda^2 I \), and has a filtered SVD expansion

\[
x_\lambda = \sum_{i=1}^{n} f_i \frac{u_i^T b}{\sigma_i} v_i,
\]

where the \( f_i = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2} \) are called filters. The error \( x_\lambda - x_{\text{true}} \) can be written as the sum of the regularization and perturbation errors, and an optimal \( \lambda_{\text{opt}} \) is such that \( \| x_{\text{true}} - x_{\text{opt}} \| = \min_{\lambda \geq 0} \| x_{\text{true}} - x_\lambda \| \) and balances these two errors [33, 36, 53, 87]. In the spirit of \( x_{\text{opt}} \), the best Tikhonov regularized solution \( x_{\text{opt}} \) retains the \( k_0 \) dominant SVD components and dampens the other \( n - k_0 \) small SVD components as much as possible [33, 36], that is, \( \lambda_{\text{opt}} \) must be such that \( f_i = \mathcal{O}(1) \) for \( i = 1, 2, \ldots, k_0 \) and \( f_i/\sigma_i \approx 0 \) for \( i = k_0 + 1, \ldots, n \). Therefore, it is expected that \( x_{k_0} \) and \( x_{\text{opt}} \) have very similar accuracy. This is indeed true. Actually, it has been observed and
justified that these two regularized solutions essentially have the minimum 2-norm error; see [31], [33, p.109-11], and [36, Sections 4.2 and 4.4], and [85].

As a matter of fact, there is solid mathematical theory on the TSVD method and standard-form Tikhonov regularization: for an underlying linear compact equation $Kx = g$, e.g., (1.2), with the noisy $g$ and true solution $x_{\text{true}}$, under the source condition that its solution $x_{\text{true}} \in \mathcal{R}(K^*)$ or $x_{\text{true}} \in \mathcal{R}(K^*K)$, the range of the adjoint $K^*$ of $K$ or that of $K^*K$, the errors of $x_{\text{tsvd}}$ and $x_{\lambda_{\text{opt}}}$ are order optimal, i.e., the same order as the worst-case error [53, p.13,18,20,32-40], [60, p.90] and [87, p.7-12]. These conclusions carries over to (1.1) [87, p.8]. Therefore, both $x_{\lambda_{\text{opt}}}$ and $x_{\text{tsvd}}$ are best possible solutions to (1.1) under the above assumptions. More generally, for $x_{\text{true}} \in \mathcal{R}((K^*K)^{\beta/2})$ with any $\beta > 0$, the error of the TSVD solution $x_{\text{tsvd}}$ is always order optimal, while $x_{\lambda_{\text{opt}}}$ is best possible only for $\beta \leq 2$; see [17, Chap. 4-5] for details.

A number of parameter-choice methods have been developed for finding $\lambda_{\text{opt}}$ or $k_0$, such as the discrepancy principle [58], the L-curve criterion, whose use goes back to Miller [57] and Lawson and Hanson [55] and is termed much later and studied in detail in [32, 37], the generalized cross validation (GCV) [24, 88], and the method based on error estimation [21, 71]; see, e.g., [3, 17, 33, 36, 50, 51, 52, 62, 87] for numerous comparisons. Each of these methods has its own merits and disadvantages, and none is absolutely reliable for all discrete ill-posed problems. For example, some of them may fail to find accurate approximations to $\lambda_{\text{opt}}$; see [27, 86] for an analysis on the L-curve criterion method and [33] for some other parameter-choice methods.

As a result, we will take $x_{\text{tsvd}}$ as the reference standard when assessing the accuracy of the best regularized solution obtained by a regularization method. In other words, we take the TSVD method as reference standard to evaluate the regularization ability of a regularization method.

For $A$ large, the TSVD method and the Tikhonov regularization method are generally too demanding, and only iterative regularization methods are computationally viable. Krylov solvers are a major class of iterative methods for solving (1.1), and they project (1.1) onto a sequence of low dimensional Krylov subspaces and computes iterates to approximate $x_{\text{true}}$ [1, 17, 23, 26, 33, 36, 53]. Of them, the CGLS (or CGNR) method, which implicitly applies the CG method [25, 39] to $A^T Ax = A^T b$, and its mathematically equivalent LSQR algorithm [67] have been most commonly used. The Krylov solvers CGME (or CGNE) [8, 9, 14, 26, 28] and LSMR [9, 19] are also choices, which amount to the CG method applied to $\min \| AA^T y - b \|$ or $AA^T y = b$ with $x = A^T y$ and MINRES [66] applied to $A^T Ax = A^T b$, respectively. These Krylov solvers have been intensively studied and known to have general regularizing effects [1, 15, 23, 26, 28, 33, 36, 40, 41] and exhibit semi-convergence [60, p.89]; see also [8, p.314], [9, p.73], [13, p.135] and [36, p.110]: the iterates converge to $x_{\text{true}}$ and their norms increase steadily, and the residual norms decrease 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 $x_{\text{native}}$, while their norms increase considerably and the residual norms stabilize. 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 becomes ill conditioned from some iteration onwards, and a small singular value of the projected problem amplifies the noise considerably.

The behavior of ill-posed problems critically depends on the decay rate of $\sigma_j$. The following characterization of the degree of ill-posedness of (1.1) was introduced in [42] and has been widely used [1, 17, 33, 36, 59]: if $\sigma_j = \mathcal{O}(\rho^{-j})$ with $\rho > 1$,
$j = 1, 2, \ldots, n$, then (1.1) is severely ill-posed; if $\sigma_j = O(j^{-\alpha})$, then
(1.1) is mildly or moderately ill-posed for $\frac{1}{2} < \alpha \leq 1$ or $\alpha > 1$. Here for mildly ill-posed problems
we add the requirement $\alpha > \frac{1}{2}$, which does not appear in [42] but must be met for a
linear compact operator equation [29, 33].

The regularizing effects of CG type methods were discovered in [48, 74, 78]. Johnson
[48] had given a heuristic explanation on the success of CGLS. Based on these
works, on page 13 of [10], Björck and Eldén in their 1979 survey 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 [33, p.145]. As remarked by Hanke and Hansen [29], the paper [10] was the
only extensive survey on algorithmic details until that time. Hanke and Hansen [29]
and Hansen [34] have addressed that a strict proof of the regularizing properties of
conjugate gradients is extremely difficult.

An enormous effort has been made to the study of regularizing effects of LSQR
and CGLS; see [18, 22, 26, 28, 33, 36, 40, 41, 43, 61, 64, 68, 73, 82], many of which
concern the asymptotic behavior of the errors of $x_{\lambda, opt}$ and $x_{k_{0}}^{tsvd}$ as the noise $e$, which
is not required to possess any property, approaches zero in the Hilbert, i.e., infinite
dimensional, space setting. Our concern is to leave the white noise $e$ fixed and conside-
rs how the solution by LSQR and CGLS behaves as the regularization parameter
varies in the finite dimensional space, so our analysis approach and results are non-
asymptotic and different. It has long been well known [29, 33, 34, 36] and will also be
elaborated in this paper that provided that the Ritz values involved in LSQR always
approximate the large singular values of $A$ in natural order until semi-convergence, the
best regularized solution obtained by LSQR is as accurate as $x_{k_{0}}^{tsvd}$. Such convergence
is thus desirable. Hansen [33, 34, 36] and many others, e.g., Gazzola and Novati [20],
address the difficulties to prove the convergence in this order. As a matter of fact,
hitherto there has been no general definitive and quantitative result on whether or not
the Ritz values converge in this order. As a matter of fact, it is well possible
that the Ritz values fail to converge to the large singular values of $A$ in natural order
for some ill-posed problems, as will be reported in this paper. In this case, nothing
has been known how well LSQR works, namely, how accurate the best regularized
solution by LSQR is.

If a regularized solution to (1.1) is as accurate as $x_{k_{0}}^{tsvd}$, then it is called a best
possible regularized solution. If the regularized solution by an iterative 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 has been unknown whether or not LSQR, CGLS, LSMR, and CGME have
the full regularization for a given (1.1), one commonly combines them with some ex-
licit regularization, hoping that the resulting (hybrid) variants can find best possible
regularized solutions [1, 33, 36]. CGLS is combined with the standard-form Tikhonov
regularization, and it solves $(A^{T}A + \lambda^{2}I)x = A^{T}b$ for several trial regularization pa-
rameters $\lambda$ and picks up the best one among the candidates [1]. The hybrid LSQR
variants have been advocated by Björck and Eldén [10] and O’Leary and Simmons
[65], and improved and developed by Björck [7], Björck, Grimme and van Dooren [11],
and Renaut, Vatankhah, and Ardeshani [72]. They first project (1.1) onto Krylov sub-
spaces and then regularize the projected problem explicitly at each iteration. They
aim to remove the effects of small Ritz values and expands Krylov subspaces until
they captures the $k_{0}$ dominant SVD components of $A$. The hybrid LSQR, CGME
and LSMR have been intensively studied in, e.g., [4, 5, 6, 12, 13, 28, 29, 56, 63, 72]
If an iterative solver is theoretically proved and practically identified to have the full regularization, then, in principle, one simply stops it after a few iterations of semi-convergence, and no complicated hybrid variant is needed. Obviously, we cannot emphasize too much the importance of proving the full or partial regularization of LSQR, CGLS, LSMR and CGME. To echo the concern of Björck and Eldén, by the definition of the full or partial regularization, our fundamental question is: Do LSQR, CGLS, LSMR and CGME have the full or partial regularization for severely, moderately and mildly ill-posed problems? In view of our previous description, there has been no definitive answer to this long-standing fundamental question hitherto.

LSQR (or CGLS), CGME and LSMR are common in that, at iteration \( k \), they all are mathematically based on the same \( k \)-step Lanczos bidiagonalization process and compute different iterates from the same \( k \)-dimensional Krylov subspace. Remarkably, note that if the left and right subspaces are the \( k \) dimensional dominant left and right singular subspaces \( \text{span} \{ U_k \} \) and \( \text{span} \{ V_k \} \) of \( A \) then the Ritz values of \( A \) with respect to them are exactly the first \( k \) large singular values of \( A \). Therefore, whether or not the Ritz values converge to the large singular values of \( A \) in natural order critically depends on how the underlying \( k \)-dimensional Krylov subspace approaches \( \text{span} \{ V_k \} \). This paper concerns a common and fundamental problem that these methods face: how accurately does the underlying \( k \)-dimensional Krylov subspace approximate \( \text{span} \{ V_k \} \)? Accurate solutions of this problem play a central role in analyzing the regularization ability of the mentioned four methods and in ultimately determining if each method has the full regularization. We will, for the first time, establish a general \( \sin \Theta \) theorem for the 2-norm distances between these two subspaces, derive accurate estimates on them for the three kinds of ill-posed problems, and show how the Krylov subspace approximates \( \text{span} \{ V_k \} \). We will notice that the \( \sin \Theta \) theorem involves some crucial quantities that are used to studying the regularizing effects of LSQR [33, p.150-2], but there were no estimates for them there and in the literature.

In Section 2, we describe the Lanczos bidiagonalization process and the LSQR, CGME and LSMR methods, and make an introductory analysis by taking LSQR as example. In Section 3 we make an analysis on the regularizing effects of LSQR and establish a basic result on its semi-convergence. In Section 4, we establish the \( \sin \Theta \) theorem for the 2-norm distance between the underlying \( k \)-dimensional Krylov subspace and \( \text{span} \{ V_k \} \), and derive accurate estimates on them for the three kinds of ill-posed problems, which include accurate estimates for those key quantities in [33, p.150-2]. In Section 5 we give a manifestation of the \( \sin \Theta \) theorem on the behavior of the smallest Ritz values involved in LSQR. We report numerical examples to confirm our theory and illustrate that our estimates are sharp. Finally, we summarize the paper in Section 6.

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 the bold letter \( \mathbf{0} \) the identity matrix and the zero matrix with orders clear from the context, respectively. For the matrix \( B = (b_{ij}) \), we define \( |B| = (|b_{ij}|) \), and for \( |C| = (|c_{ij}|) \), \(|B| \leq |C|\) means \(|b_{ij}| \leq |c_{ij}|\) componentwise.

2. The LSQR, CGME and LSMR algorithms. These three algorithms are based on the same Lanczos bidiagonalization process, which computes two orthonormal bases \( \{q_1, q_2, \ldots, q_k\} \) and \( \{p_1, p_2, \ldots, p_{k+1}\} \) of \( K_k(A^T A, A^T b) \) and \( K_{k+1}(AA^T, b) \) for \( k = 1, 2, \ldots, n \), respectively. We describe the process as Algorithm 1.
Algorithm 1: k-step Lanczos bidiagonalization process

- Take \( p_1 = b/\|b\| \in \mathbb{R}^m \), and define \( \beta_1 q_0 = 0 \) with \( \beta_1 = \|b\| \).
- 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) \( \beta_{j+1} = \|z\| ; p_{j+1} = z/\beta_{j+1} \).

Algorithm 1 can be written in the matrix form

\[
(AQ_k)_{k+1}B_k, \\
(A^TP_{k+1}) = Q_kB_k^T + \alpha_{k+1}q_{k+1}(e_{k+1}^{(k+1)})^T,
\]

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

\[
B_k = \begin{pmatrix}
\alpha_1 & \alpha_2 & \beta_3 & \cdots & \beta_k & \alpha_k \\
\beta_2 & \beta_3 & \cdots & \beta_k & \beta_{k+1}
\end{pmatrix} \in \mathbb{R}^{(k+1) \times k}.
\]

It is known from (2.1) that

\[
B_k = P_{k+1}^T AQ_k.
\]

Algorithm 1 cannot break down before step \( n \) when \( \sigma_i, i = 1, 2, \ldots, n \), are simple since \( b \) has nonzero components in the directions of \( u_i, i = 1, 2, \ldots, n \). 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 \( \text{span}\{P_{k+1}\} \) and \( \text{span}\{Q_k\} \), are all simple as \( \alpha_i > 0, \beta_{i+1} > 0, i = 1, 2, \ldots, k \).

Write \( k(A^TA, A^Tb) = V_k^{R} \) and \( \mathcal{V}_k = \text{span}\{V_k\} \). At iteration \( k \), LSQR [67] solves the problem

\[
\|Ax_k^{lsqr} - b\| = \min_{x \in \mathcal{V}_k} \|Ax - b\|
\]

for the iterate

\[
x_k^{lsqr} = Q_ky_k^{lsqr} \quad \text{with} \quad y_k^{lsqr} = \arg \min_{y \in \mathbb{R}^k} \|B_ky - \beta_1e_1^{(k+1)}\| = \beta_1B_k^Te_1^{(k+1)},
\]

where \( e_1^{(k+1)} \) is the first canonical basis vector of \( \mathbb{R}^{k+1} \), and the residual norm \( \|Ax_k^{lsqr} - b\| = \|B_ky_k^{lsqr} - \beta_1e_1^{(k+1)}\| \) decreases monotonically with respect to \( k \).

CGME [9, 26, 28, 40, 41] is the CG method applied to \( \min \|AA^Ty - b\| \) or \( AA^Ty = b \) and \( x = A^T y \), and it solves the problem

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

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

\[
\bar{B}_k = P_k^T AQ_k.
\]
Then
\begin{equation}
(2.7) \\
x_k^{\text{cgme}} = Q_k y_k^{\text{cgme}} \quad \text{with} \quad y_k^{\text{cgme}} = \beta_1 \tilde{B}_k^{-1} e_1^{(k)}
\end{equation}
and the residual norm \(\| A x_k^{\text{cgme}} - b \| = \beta_{k+1} |(e_k^{(k)})^T y_k^{\text{cgme}}| \) with \( e_1^{(k)} \) and \( e_k^{(k)} \) the first
and the \( k \)-th canonical vectors of dimension \( k \), respectively.

LSMR [9, 19] is mathematically equivalent to MINRES [66] applied to the normal equation \( A^T A x = A^T b \), and it solves
\[
\| A^T (b - A x_k^{\text{lsmr}}) \| = \min_{x \in \mathbb{R}^k} \| A^T (b - A x) \|
\]
for the iterate \( x_k^{\text{lsmr}} \). The residual norm \( \| A^T (b - A x_k^{\text{lsmr}}) \| \) of the normal equation decreases monotonically with respect to \( k \), and
\begin{equation}
(2.8) \\
x_k^{\text{lsmr}} = Q_k y_k^{\text{lsmr}} \quad \text{with} \quad y_k^{\text{lsmr}} = \arg \min_{y \in \mathbb{R}^k} \| (B_k^T B_k, \alpha_{k+1} \beta_k e_k)^T y - \alpha_1 \beta_1 e_1^{(k+1)} \|.
\end{equation}

As we have seen, the iterates \( x_k^{\text{lsmr}}, x_k^{\text{cgme}} \) and \( x_k^{\text{lsmr}} \) are different but they are all extracted from \( Y_k \). We now take LSQR as example and give an insightful illustration in order to introduce the problems that must be solved for answering the open question on its full or partial regularization. From \( \beta_1 e_1^{(k+1)} = P_{k+1}^T b \) and (2.5), we have
\begin{equation}
(2.9) \\
x_k^{\text{lsqr}} = Q_k B_k^T P_{k+1}^T b,
\end{equation}
that is, \( x_k^{\text{lsqr}} \) is the minimum 2-norm solution to the perturbed problem that replaces \( A \) in (1.1) by its rank \( k \) approximation \( P_{k+1} B_k Q_k^T \). So LSQR solves
\begin{equation}
(2.10) \\
\min \| x \| \quad \text{subject to} \quad \| P_{k+1} B_k Q_k^T x - b \| = \min
\end{equation}
for the regularized solutions \( x_k^{\text{lsqr}} \) to (1.1) starting with \( k = 1 \) onwards. Recall the TSVD method (cf. (1.9)) and that the best rank \( k \) approximation \( A_k \) to \( A \) satisfies \( \| A - A_k \| = \sigma_{k+1} \). Consequently, if \( P_{k+1} B_k Q_k^T \) is a near best rank \( k \) approximation to \( A \) with an approximate accuracy \( \sigma_{k+1} \) and the \( k \) singular values of \( B_k \) approximate the first \( k \) large ones of \( A \) in natural order for \( k \leq k_0 \), then LSQR and the TSVD method are related naturally and closely because (i) \( x_k^{\text{svd}} \) and \( x_k^{\text{lsqr}} \) are the regularized solutions to the two perturbed problems of (1.1) that replace \( A \) by its two rank \( k \) approximations with the same quality, respectively; (ii) \( x_k^{\text{svd}} \) and \( x_k^{\text{lsqr}} \) solve the two essentially same regularization problems (1.9) and (2.10), respectively. As a consequence, the LSQR iterate \( x_k^{\text{lsqr}} \) is as accurate as \( x_k^{\text{svd}} \), and LSQR has the full regularization. Therefore, that \( P_{k+1} B_k Q_k^T \) is a near best rank \( k \) approximation to \( A \) and the \( k \) singular values of \( B_k \) approximate the large ones of \( A \) in natural order for \( k \leq k_0 \) is sufficient conditions for LSQR having the full regularization.

However, we must remind that the near best rank \( k \) approximations and the approximations of the singular values of \( B_k \) to the large \( \sigma_i \) in natural order may not be necessary conditions for the full regularization of LSQR.

3. Some arguments and results on the regularizing effects of LSQR.
The following result (cf., e.g., van der Sluis and van der Vorst [81]) has been widely used, e.g., in Hansen [33] to illustrate the regularizing effects of LSQR and CGLS.

**Proposition 3.1.** LSQR with the starting vector \( p_1 = b/\| b \| \) and CGLS applied to \( A^T A x = A^T b \) with the zero starting vector generate the same iterates
\begin{equation}
(3.1) \\
x_k^{\text{lsqr}} = \sum_{i=1}^{n} f_i^{(k)} \frac{y_i^T b}{\sigma_i} v_i, \quad k = 1, 2, \ldots, n,
\end{equation}
where the filters

\[
 f_i^{(k)} = 1 - \prod_{j=1}^{k} \frac{(\theta_j^{(k)})^2 - \sigma_i^2}{(\theta_j^{(k)})^2}, \quad i = 1, 2, \ldots, n,
\]

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

It is seen from (3.1)–(3.2) that $x_{\text{l}sqr}^\ast$ has a filtered SVD expansion. If all the Ritz values $\theta_j^{(k)}$ approximate the large singular values $\sigma_j$ of $A$ in natural order, the filters $f_i^{(k)} \approx 1$ for $i = 1, 2, \ldots, k$ and $f_i^{(k)}$ monotonically approach zero for $i = k + 1, \ldots, n$. This indicates that if the $\theta_j^{(k)}$ approximate the first $k$ singular values $\sigma_j$ of $A$ in natural order for $k = 1, 2, \ldots, k_0$ then LSQR definitely has the full regularization.

Applying the Cauchy’s strict interlacing theorem [77, p.198, Corollary 4.4] to the singular values of $B_k$ and $B_n$, it always holds that

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

independent of the degree of ill-posedness of (1.1). Therefore, at iteration $k_0 + 1$ one must have $\theta_{k_0+1}^{(k_0+1)} < \sigma_{k_0+1}$. By (3.1) and (3.2), we have $f_{k_0+1}^{(k_0+1)} \approx 1$, meaning that $x_{\text{l}sqr}^\ast$ must already be deteriorated. Therefore, the semi-convergence of LSQR occurs no later than iteration $k_0$.

If the $\theta_j^{(k)}$ do not converge to the large singular values of $A$ in natural order and $\theta_k^{(k)} < \sigma_{k_0+1}$ before some iteration $k < k_0$, then $x_{\text{l}sqr}^\ast$ is already deteriorated by the noise $\varepsilon$ before such $k$: suppose that $\sigma_{j^*} < \theta_k^{(k)} < \sigma_{k_0+1}$ at iteration $k$ with $j^*$ the smallest integer $j^* > k_0 + 1$. Then we can easily justify from (3.2) that $f_i^{(k)} \in (0, 1)$ tends to zero monotonically for $i = j^*, j^* + 1, \ldots, n$, but we have

\[
 \prod_{j=1}^{k} \frac{(\theta_j^{(k)})^2 - \sigma_i^2}{(\theta_j^{(k)})^2} \prod_{j=1}^{k-1} \frac{(\theta_j^{(k)})^2 - \sigma_i^2}{(\theta_j^{(k)})^2} \leq 0, \quad i = k_0 + 1, \ldots, j^* - 1
\]

since the first factor is non-positive and the second factor is positive. Hence $f_i^{(k)} \geq 1$ for $i = k_0 + 1, \ldots, j^* - 1$, meaning that $x_{\text{l}sqr}^\ast$ has been deteriorated by the noise $\varepsilon$ and the semi-convergence of LSQR has occurred at some iteration $k^* < k$.

On the other hand, if $k^* < k_0$, then the $k^*$ Ritz values $\theta_i^{(k^*)}$ must not approximate the large singular values of $A$ in natural order; otherwise, since $\theta_i^{(k^*)} \in (\sigma_{k^*+1}, \sigma_{k^*})$ means $\theta_i^{(k^*)} > \sigma_{k_0}$, this, by the above analysis, indicates that the semi-convergence of LSQR does not yet occur and $x_{\text{l}sqr}^\ast$ can be further improved in the next iteration.

Summarizing the above, we have proved the following basic and important result.

**Theorem 3.1.** 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 $k^* < k_0$, and vice versa.

If the semi-convergence of LSQR occurs at iteration $k^* < k_0$, the regularizing effects of LSQR is much more involved and complicated, and there has been no general result on the full or partial regularization of LSQR. This problem will be our future concern.
The standard $k$-step Lanczos bidiagonalization method [8, 9] that computes the $k$ Ritz values $\theta_i^{(k)}$ is mathematically equivalent to the symmetric Lanczos method for the eigenvalue problem of $A^TA$ starting with $q_1 = A^Tb/\|A^Tb\|$; see [2, 8, 9, 69, 83] or [46, 47] for several variations that are based on standard, harmonic, and refined projection [2, 76, 83] or a combination of them [45]. An attractive feature is that, for general singular value distribution and the vector $b$, some Ritz values become good approximations to the extreme singular values of $A$ as $k$ increases. If large singular values are well separated but small singular values are clustered, large Ritz values converge fast but small Ritz values show up late and converge slowly.

For (1.1), since the singular values $\sigma_j$ of $A$ decay to zero, $A^Tb = \sum_{j=1}^{n} \sigma_j (u_j^Tb)v_j$ contains more information on dominant right singular vectors than on the ones corresponding to small singular values. Therefore, $\mathcal{V}_k^R$ with $A^Tb$ as the starting vector is expected to contain richer information on the first $k$ right singular vectors $v_j$ than on the other $n-k$ ones. Note that $A$ has many small singular values clustered at zero. Due to these two basic facts, all the $\theta_j^{(k)}$ are expected to approximate the large singular values of $A$ in natural order until some iteration $k$. In this case, the iterates $x_k^{(\text{svr})}$ mainly consists of the $k$ dominant SVD components of $A$, as we have shown. This is why LSQR and CGLS have general regularizing effects; see, e.g., [1, 33, 35, 36].

Unfortunately, the above arguments are only qualitative. As has been addressed, proving that the Ritz values converge in natural order is extremely difficult [29, 33, 34, 36]. Some numerical examples and model problems in [82, 84] have indicated that the desired convergence of the Ritz values actually holds as long as the discrete Picard condition is satisfied and there is a good separation among the large singular values of $A$. Yet, there has been no mathematical justification on these observations.

4. sin $\Theta$ theorems for the distances between $\mathcal{V}_k^R$ and $\text{span}\{V_k\}$. As can be seen from Sections 2–3, a complete understanding of the regularization of LSQR includes accurate solutions of the following problems: (i) How accurately does the $k$ dimensional Krylov subspace $\mathcal{V}_k^R$ approximate the $k$ dimensional dominant right singular subspace $\text{span}\{V_k\} = \mathcal{V}_k$ of $A$? (ii) How accurate is the rank $k$ approximation $P_{k+1}B_kQ_k^T$ to $A$? (iii) When do the $\theta_i^{(k)}$ approximate the large $\sigma_i$ in natural order? (iv) When does at least a small Ritz value appear, i.e., $\theta_i^{(k)} < \sigma_{k+1}$ for some $k \leq k^*$? (v) How to solve Problems (i)-(iii) in the case that $A$ has multiple singular values? (vi) Does LSQR have the full or partial regularization when the $k$ Ritz values $\theta_i^{(k)}$ do not approximate the large singular values of $A$ in natural order for some $k \leq k^*$? Problem (i) is the starting and key point to the other problems, and its accurate solutions form an absolutely necessary basis of dealing with the others.

In this paper, we focus on Problem (i) in detail and present accurate results, and we will also make a tentative analysis on Problem (iv). Based on the results on Problem (i), we will make an in-depth analysis on all the other problems mentioned in the follow-up work.

In terms of the canonical angles $\Theta(\mathcal{X}, \mathcal{Y})$ between two subspaces $\mathcal{X}$ and $\mathcal{Y}$ of equal dimension (cf. [76, p.74-5] and [77, p.43]), we first present a general sin $\Theta$ theorem which measures the 2-norm distance between $\mathcal{V}_k$ and $\mathcal{V}_k^R$, and then prove how $\mathcal{V}_k^R$ approximates $\mathcal{V}_k$ for severely ill-posed problems.

**Theorem 4.1.** For $k = 1, 2, \ldots, n-1$ we have

\[
\| \sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R) \| = \frac{\| \Delta_k \|}{\sqrt{1 + \| \Delta_k \|^2}}
\]
with $\Delta_k \in \mathbb{R}^{(n-k) \times k}$ to be defined by (4.7). Let the SVD of $A$ be as (1.5). Assume that (1.1) is severely ill-posed with $\sigma_j = O(\rho^{-j})$ and $\rho > 1$, $j = 1, 2, \ldots, n$, and the discrete Picard condition (1.7) is satisfied. Then

\begin{equation}
\|\Delta_1\| \leq \frac{\sigma_2}{\sigma_1} \frac{|u_1^T b|}{|u_1^T b|} (1 + O(\rho^{-2})) ,
\end{equation}

\begin{equation}
\|\Delta_k\| \leq \frac{\sigma_{k+1}}{\sigma_k} \frac{|u_{k+1}^T b|}{|u_k^T b|} (1 + O(\rho^{-2})) |L_{k_1}^{(k)}(0)|, \quad k = 2, 3, \ldots, n - 1,
\end{equation}

where

\begin{equation}
|L_{k_1}^{(k)}(0)| = \max_{j=1,2,\ldots,k} |L_j^{(k)}(0)|, \quad |L_j^{(k)}(0)| = \prod_{i=1, i \neq j}^k \frac{\sigma_2}{|\sigma_j - \sigma_i|}, \quad j = 1, 2, \ldots, k.
\end{equation}

Proof. Let $U_n = (u_1, u_2, \ldots, u_n)$ whose columns are the first $n$ left singular vectors of $A$ defined by (1.5). Then the Krylov subspace $K_k(\Sigma^{2}, \Sigma U_n^T b) = \text{span}\{DT_k\}$ with

\begin{equation}
D = \text{diag}(\sigma_i u_i^T b) \in \mathbb{R}^{n \times n}, \quad T_k = \begin{pmatrix} 1 & \sigma_1^2 & \ldots & \sigma_1^{2k-2} \\ 1 & \sigma_2^2 & \ldots & \sigma_2^{2k-2} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \sigma_n^2 & \ldots & \sigma_n^{2k-2} \end{pmatrix}.
\end{equation}

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

\begin{equation}
D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix}, \quad T_k = \begin{pmatrix} T_{k1} \\ T_{k2} \end{pmatrix},
\end{equation}

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 $K_k(A^T A, A^T b) = \text{span}\{VDT_k\}$ we have

\begin{equation}
V_k^R = K_k(A^T A, A^T b) = \text{span}\{V \left( \begin{array}{c} D_1 T_{k1} \\ D_2 T_{k2} \end{array} \right) \} = \text{span}\{V \left( \begin{array}{c} I \\ \Delta_k \end{array} \right) \},
\end{equation}

where

\begin{equation}
\Delta_k = D_2 T_{k2} T_{k1}^{-1} D_1^{-1} \in \mathbb{R}^{(n-k) \times k}.
\end{equation}

Write $V = (V_k, V_k^\perp)$, and define

\begin{equation}
Z_k = V \left( \begin{array}{c} I \\ \Delta_k \end{array} \right) = V_k + V_k^\perp \Delta_k.
\end{equation}

Then $Z_k^T Z_k = I + \Delta_k^T \Delta_k$, and the columns of $\hat{Z}_k = Z_k(Z_k^T Z_k)^{-\frac{1}{2}}$ form an orthonormal basis of $V_k^R$. As a result, we get an orthogonal direct sum decomposition

\begin{equation}
\hat{Z}_k = (V_k + V_k^\perp \Delta_k)(I + \Delta_k^T \Delta_k)^{-\frac{1}{2}}.
\end{equation}

By the definition of $\Theta(V_k, V_k^R)$ and (4.9), we obtain

\begin{equation}
\|\sin(\Theta(V_k, V_k^R))\| = \|V_k^R^T Z_k\| = \|\Delta_k(I + \Delta_k^T \Delta_k)^{-\frac{1}{2}}\| = \frac{\|\Delta_k\|}{\sqrt{1 + \|\Delta_k\|^2}}.
\end{equation}
which proves (4.1).

Next we estimate $\|\Delta_k\|$. For $k = 2, 3, \ldots, n - 1$, it is easily justified that the $j$-th column of $T_{k1}^{-1}$ consists of the coefficients of the $j$-th Lagrange polynomial

$$L_j^{(k)}(\lambda) = \prod_{i=1, i \neq j}^k \frac{\lambda - \sigma_i^2}{\sigma_j^2 - \sigma_i^2}$$

that interpolates the elements of the $j$-th canonical basis vector $e_j^{(k)} \in \mathbb{R}^k$ at the abscissas $\sigma_1^2, \sigma_2^2, \ldots, \sigma_k^2$. Consequently, the $j$-th column of $T_{k2}T_{k1}^{-1}$ is

$$T_{k2}T_{k1}^{-1} e_j^{(k)} = (L_j^{(k)}(\sigma_{k+1}^2), \ldots, L_j^{(k)}(\sigma_n^2))^T, \ j = 1, 2, \ldots, k,$$

from which we obtain

$$T_{k2}T_{k1}^{-1} = \begin{pmatrix}
L_1^{(k)}(\sigma_{k+1}^2) & L_2^{(k)}(\sigma_{k+1}^2) & \cdots & L_k^{(k)}(\sigma_{k+1}^2) \\
L_1^{(k)}(\sigma_{k+2}^2) & L_2^{(k)}(\sigma_{k+2}^2) & \cdots & L_k^{(k)}(\sigma_{k+2}^2) \\
\vdots & \vdots & \ddots & \vdots \\
L_1^{(k)}(\sigma_n^2) & L_2^{(k)}(\sigma_n^2) & \cdots & L_k^{(k)}(\sigma_n^2)
\end{pmatrix} \in \mathbb{R}^{(n-k)\times k}.$$

Since $|L_j^{(k)}(\lambda)|$ is monotonically decreasing for $0 \leq \lambda < \sigma_k^2$, it is bounded by $|L_j^{(k)}(0)|$. With this property and the definition of $L_{k1}^{(k)}(0)$, we obtain

$$|\Delta_k| = |D_2T_{k2}T_{k1}^{-1}D_1^{-1}| \leq \begin{pmatrix}
\sigma_{k+1}/\sigma_1 & u_{k+1}^T b/L_{k1}^{(k)}(0) & u_{k+1}^T b/L_{k1}^{(k)}(0) & \cdots & u_{k+1}^T b/L_{k1}^{(k)}(0) \\
\sigma_{k+2}/\sigma_1 & u_{k+2}^T b/L_{k1}^{(k)}(0) & u_{k+2}^T b/L_{k1}^{(k)}(0) & \cdots & u_{k+2}^T b/L_{k1}^{(k)}(0) \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\sigma_k/\sigma_1 & u_k^T b/L_{k1}^{(k)}(0) & u_k^T b/L_{k1}^{(k)}(0) & \cdots & u_k^T b/L_{k1}^{(k)}(0)
\end{pmatrix}$$

$$= |L_{k1}^{(k)}(0)||\tilde{\Delta}_k|,$$

where

$$|\tilde{\Delta}_k| = \left|\frac{\sigma_{k+1}u_{k+1}^T b, \sigma_{k+2}u_{k+2}^T b, \ldots, \sigma_n u_n^T b}{}\right|$$

is a rank one matrix. Therefore, by $||C|| \leq ||C||$ (cf. [75, p.53]), we have

$$||\Delta_k|| \leq ||\Delta_k|| \leq |L_{k1}^{(k)}(0)|||\tilde{\Delta}_k||$$

$$= |L_{k1}^{(k)}(0)|\left(\sum_{j=k+1}^n \sigma_j^2|u_j b|^2\right)^{1/2} \left(\sum_{j=1}^k \frac{1}{\sigma_j^2|u_j b|^2}\right)^{1/2}.$$

By the discrete Picard condition (1.7), (1.8) and the properties on the white noise $e$, it is known from [33, p.70-1] and [36, p.41-2] that $|u_j^T b| \approx |u_j^T b_{true}| = \sigma_j^{1+b}$ decreases as $j$ increases up to $k_0$ and then become stabilized as $|u_j^T b| \approx |u_j^T e| \approx \eta$ for
\[ j > k_0. \] So, in order to simplify the derivation and present our results compactly, in later proofs we will use the following ideal strict equalities and inequalities:

\begin{align*}
(4.15) & \quad |u_j^T b| = |u_j^T b_{\text{true}}| = \sigma_j^{1+\beta}, \quad j = 1, 2, \ldots, k_0, \\
(4.16) & \quad |u_j^T b| = |u_j^T e| = \eta, \quad j = k_0 + 1, \ldots, n, \\
(4.17) & \quad |u_{j+1}^T b| \leq |u_j^T b|, \quad j = 1, 2, \ldots, n - 1.
\end{align*}

From (4.17) and \( \sigma_j = O(\rho^{-j}), \quad j = 1, 2, \ldots, n, \) for \( k = 1, 2, \ldots, n - 1 \) we obtain

\begin{align*}
& \left( \sum_{j=k+1}^{n} \sigma_j^2 |u_j^T b|^2 \right)^{1/2} = \sigma_{k+1} |u_{k+1}^T b| \left( \sum_{j=k+1}^{n} \frac{\sigma_j^2 |u_j^T b|^2}{\sigma_{k+1}^2 |u_{k+1}^T b|^2} \right)^{1/2} \\
& \leq \sigma_{k+1} |u_{k+1}^T b| \left( \sum_{j=k+1}^{n} \frac{\sigma_j^2}{\sigma_{k+1}^2} \right)^{1/2} \\
& = \sigma_{k+1} |u_{k+1}^T b| \left( 1 + \sum_{j=k+2}^{n} O(\rho^{2(k-j)+2}) \right)^{1/2} \\
& = \sigma_{k+1} |u_{k+1}^T b| \left( 1 + O \left( \sum_{j=k+2}^{n} \rho^{2(k-j)+2} \right) \right)^{1/2} \\
& = \sigma_{k+1} |u_{k+1}^T b| \left( 1 + O \left( \frac{\rho^{-2}}{1 - \rho^{-2}} (1 - \rho^{-2(n-k-1)}) \right) \right)^{1/2} \\
& = \sigma_{k+1} |u_{k+1}^T b| \left( 1 + O(\rho^{-2}) \right)^{1/2} \\
& = \sigma_{k+1} |u_{k+1}^T b| \left( 1 + O(\rho^{-2}) \right)
\end{align*}

with \( 1 + O(\rho^{-2}) = 1 \) for \( k = n - 1. \) For \( k = 2, 3, \ldots, n - 1, \) from (4.17) we get

\begin{align*}
& \left( \sum_{j=1}^{k} \frac{1}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2} = \frac{1}{\sigma_k |u_k^T b|} \left( \sum_{j=1}^{k} \frac{\sigma_j^2 |u_j^T b|^2}{\sigma_k^2 |u_k^T b|^2} \right)^{1/2} \leq \frac{1}{\sigma_k |u_k^T b|} \left( \sum_{j=1}^{k} \frac{\sigma_j^2}{\sigma_k^2} \right)^{1/2} \\
& = \frac{1}{\sigma_k |u_k^T b|} \left( 1 + O \left( \sum_{j=1}^{k-1} \rho^{2(j-k)} \right) \right)^{1/2} \\
& = \frac{1}{\sigma_k |u_k^T b|} (1 + O(\rho^{-2})).
\end{align*}

From the above and (4.14), we finally obtain (4.3) by noting

\[ \| \Delta_k \| \leq \frac{\sigma_{k+1} |u_{k+1}^T b|}{\sigma_k |u_k^T b|} (1 + O(\rho^{-2})) |L_k^{(k)}(0)|, \quad k = 2, 3, \ldots, n - 1. \]

Note that the Lagrange polynomials \( L_j^{(k)}(\lambda) \) require \( k \geq 2. \) So, we need to treat the case \( k = 1 \) separately. Observe from (4.7) and (4.17) that

\[ T_{k2} = (1, 1, \ldots, 1)^T, \quad D_2 T_{k2} = (\sigma_2 u_2^T b, \sigma_3 u_3^T b, \ldots, \sigma_n u_n^T b)^T, \quad T_{k1}^{-1} = 1, \quad D_1^{-1} = \frac{1}{\sigma_1 u_1^T b}. \]
Therefore, we have
\begin{equation}
\Delta_1 = (\sigma_2 u_2^T b, \sigma_3 u_3^T b, \ldots, \sigma_n u_n^T b)^T \frac{1}{\sigma_1 u_1^T b},
\end{equation}
from which and (4.18) it is direct to get (4.2).
(4.1) has been established in [43, Theorem 2.1], and we include the proof for completeness. A crucial step in proving (4.2)–(4.4) is to derive (4.12)–(4.13) and then bound the resulting \textit{rank one} matrix accurately. Huang and Jia [43] simply bounded
\[ \|\Delta_k\| \leq \|\Delta_k\|_F \leq \|D_2\| T_{k_2} T_{k_1}^{-1} \|D_1^{-1}\| \]
with \(\| \cdot \|_f\) the F-norm of a matrix, which led to a too much overestimate
\[ \|\Delta_k\| \leq \frac{\sigma_{k+1}}{\sigma_k} \frac{|u_{k+1}^T b|}{|u_k^T b|} \sqrt{k(n-k)} |L_{k_1}^{(k)}(0)|. \]

\textbf{Remark 4.1.} \(\|\Delta_k\| \) and \( |L_{j}^{(k)}(0)|, \ j = 1, 2, \ldots, k \)\ are used to study the regularizing effects of LSQR in [33, p. 150–2], but there were no estimates for themselves.

\textbf{Theorem 4.2.} For the severely ill-posed problem and \( k = 2, 3, \ldots, n-1 \), we have
\begin{align}
|L_{j}^{(k)}(0)| &= 1 + \mathcal{O}(\rho^{-2}), \\
|L_{j}^{(k)}(0)| &= \frac{1}{\prod_{i=j+1}^k \left(\frac{\sigma_i}{\sigma_j}\right)^2} \frac{1 + \mathcal{O}(\rho^{-2})}{\mathcal{O}(\rho^{-(k-j)(k-j+1)})}, \ j = 1, 2, \ldots, k - 1, \\
|L_{k_1}^{(k)}(0)| &= \max_{j=1, 2, \ldots, k} |L_{j}^{(k)}(0)| = 1 + \mathcal{O}(\rho^{-2}).
\end{align}

\textbf{Proof.} Exploiting the Taylor series expansion and \( \sigma_i = \mathcal{O}(\rho^{-i}) \) for \( i = 1, 2, \ldots, n \), by definition, for \( j = 1, 2, \ldots, k - 1 \) we have
\begin{equation}
|L_{j}^{(k)}(0)| = \prod_{i=1, i\neq j}^k \left| \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} \right| = \prod_{i=1}^{j-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} \cdot \prod_{i=j+1}^k \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} = \frac{1}{\prod_{i=j+1}^k \left(1 - \mathcal{O}(\rho^{-2(i-j)})\right)} \prod_{i=j}^k \frac{1}{\mathcal{O}(\rho^{2(i-j)})} = \frac{1}{\prod_{i=j+1}^k \mathcal{O}(\rho^{2(i-j)})} \left(1 + \sum_{i=1}^j \mathcal{O}(\rho^{-2i})\right) \left(1 + \sum_{i=1}^{k-j+1} \mathcal{O}(\rho^{-2i})\right) = \prod_{i=j+1}^k \mathcal{O}(\rho^{2(i-j)})
\end{equation}
by absorbing the higher order terms into \( \mathcal{O}(\cdot) \) in the numerator. For \( j = k \), we get
\begin{align}
|L_{k}^{(k)}(0)| &= \prod_{i=1}^k \left| \frac{\sigma_i^2}{\sigma_i^2 - \sigma_k^2} \right| = \prod_{i=1}^{k-1} \frac{1}{\mathcal{O}(\rho^{-2(k-i)})} = \prod_{i=1}^k \frac{1}{\mathcal{O}(\rho^{-2i})} = 1 + \mathcal{O}(\rho^{-2}) = 1 + \mathcal{O}\left(\frac{\rho^{-2}}{1 - \rho^{-2k}}\right) = 1 + \mathcal{O}(\rho^{-2}),
\end{align}
Therefore, for any $k$ we have
\[ 1 + \sum_{i=1}^{j} \mathcal{O}(\rho^{-2i}) = 1 + \mathcal{O}\left(\sum_{i=1}^{j} \rho^{-2i}\right) = 1 + \mathcal{O}\left(\frac{\rho^{-2}}{1 - \rho^{-2}}(1 - \rho^{-2j})\right), \]
and
\[ 1 + \sum_{i=1}^{k-j+1} \mathcal{O}(\rho^{-2i}) = 1 + \mathcal{O}\left(\sum_{i=1}^{k-j+1} \rho^{-2i}\right) = 1 + \mathcal{O}\left(\frac{\rho^{-2}}{1 - \rho^{-2}}(1 - \rho^{-2(k-j+1)})\right), \]
whose product for any $k$ is
\[ 1 + \mathcal{O}\left(\frac{2\rho^{-2}}{1 - \rho^{-2}}\right) + \mathcal{O}\left(\frac{\rho^{-2}}{1 - \rho^{-2}}\right)^2 = 1 + \mathcal{O}\left(\frac{2\rho^{-2}}{1 - \rho^{-2}}\right) = 1 + \mathcal{O}(\rho^{-2}). \]

On the other hand, note that the denominator of (4.23) is defined by
\[ \prod_{i=j+1}^{k} \left(\frac{\sigma_i}{\sigma_1}\right)^2 = \prod_{i=j+1}^{k} \mathcal{O}(\rho^{2(i-j)}) = \mathcal{O}(\rho^2 \cdots \rho^{k-j} \rho^{k-j+1}) = \mathcal{O}(\rho^k), \]
which, together with the above estimate for the numerator of (4.23), proves (4.21). Notice that the above quantity is always bigger than one for $j = 1, 2, \ldots, k - 1$. Therefore, for any $k$, combining (4.20) and (4.21) gives (4.22).

Remark 4.2. From (4.1) and (4.22), the bounds (4.2) and (4.3) are unified as
\[ (4.24) \quad \| \tan(\Theta(V_k, V_k^R)) \| = \| \Delta_k \| \leq \sigma_{k+1} |u_{k+1}^T b| |u_k^T b| (1 + \mathcal{O}(\rho^{-2})), \quad k = 1, 2, \ldots, n - 1. \]

Remark 4.3. (i) $|L_j^{(k)}(0)|$ exhibits monotonic increasing property with $j$ for a fixed $k$, and $k_1$ in (4.22) must be close to $k$; (ii) $|L_j^{(k)}(0)|$ decays monotonically with $k$ for a fixed $j$; (iii) $|L_j^{(k)}(0)|$ almost remains a constant one with $k$.

We illustrate the sharpness of (4.1) when inserting the estimates (4.2)–(4.4) into it and justify Remark 4.3. For the severely ill-posed shaw of $n = 1, 024$ from [34], whose singular values are $\sigma_i = \mathcal{O}(e^{-2i})$ with the bold $e$ the natural constant, Figure 1 (a) plots its first forty singular values computed by the Matlab built-in function svd.m. We have found that $\frac{\sigma_k}{\sigma_1} = \mathcal{O}(\epsilon_{mach})$ for $k = 21$ with the machine precision $\epsilon_{mach} = 2.22 \times 10^{-16}$, so that the computed $\sigma_k$ has no accuracy for $k \geq 21$.

The above facts tell us that it is unreliable to compute $\Delta_k$ defined by (4.7) and $\| \Delta_k \|$ because, in finite precision, we cannot compute $\mathcal{T}_{k_2}$ in (4.5) reliably due to the high inaccuracy of the computed small singular values and the possible underflows of $\sigma_i^{2j-2}$ for $i \geq 21$ and $j = 1, 2, \ldots, k$. Nevertheless, we can use Matlab built-in function subspace.m to compute the maximum of the canonical angles $\Theta(V_k, V_k^R)$ and exact $\| \sin(\Theta(V_k, V_k^R)) \|$ reliably for $k \leq 20$ once the SVD of shaw is available. We take $\rho = e^{-2}$ and compute the estimate (4.1) for $\| \sin(\Theta(V_k, V_k^R)) \|$ by taking the equalities in (4.2) and (4.3), $1 + \mathcal{O}(\rho^{-2}) = 1 + 2\rho^{-2}$ and $1 + \mathcal{O}(\rho^{-2}) |R_k^2(0)| = 1 + 3\rho^{-2}$. For $k > 1$, we use (4.4) to compute $|L_j^{(k)}(0)|$, $j = 1, 2, \ldots, k$ and $|L_k^{(k)}(0)|$. In all the tests,
we generate \( b = b_{\text{true}} + e \) with \( e = \frac{\|e\|}{\|b_{\text{true}}\|} = 10^{-3} \) and \( e \) the white noise with zero mean.

Figure 1 (b) confirms Remark 4.3 for \( k = 2, 3, \ldots, 20 \). Moreover, we see that the \( |L_{2j}^{(k)}(0)| \) become tiny swiftly for \( j \) small when \( k \) increases. Figure 1 (c) indicates that our estimates for \( \| \sin \Theta(V_k, V_k^R) \| \) match the exact ones well for \( k = 1, 2, \ldots, 15 \). We have found that the maximum and minimum of these ratios are 1.5541 and 0.8148, respectively, and the geometric mean of these ratios is 1.0629. Precisely, the ten ratios are 0.8148, 1.1458, 1.5541, 1.2825, 1.1439, 0.9972, 1.0686, 0.9562, 1.5511, 1.0015, 1.0089, 0.9666, 1.0782, 1.1439, 1.3415, 0.9662, 1.0015, 1.0089, 0.9666, 0.9662, respectively. These results demonstrate that our estimates are quite accurate and realistic. Figure 1 (d) draws the semi-convergence process of LSQR and the TSVD method, and indicates that two methods obtain the best regularized solutions at the same iterations \( k_0 = k^* = 8 \), which, from Theorem 3.1, implies that the \( k \) Ritz values \( \theta_i^{(k)} \) approximate the large singular values of \( A \) in natural order for \( k = 1, 2, \ldots, k_0 \). We will report the details in the next section.

![Fig. 1](image-url)

**Fig. 1.** (a): Partial singular values of \( \text{shaw} \); (b): plots of \( |L_{2j}^{(k)}(0)| \) for \( k = 1, 2, \ldots, 20 \); (c): the exact and estimated \( \| \sin \Theta(V_k, V_k^R) \| \); (d): the semi-convergence process of LSQR and TSVD.

Next we estimate \( \| \sin \Theta(V_k, V_k^R) \| \) for moderately and mildly ill-posed problems.

**Theorem 4.3.** For a moderately or mildly ill-posed (1.1) with \( \sigma_j = \zeta j^{-\alpha} \), \( j = 1, 2, \ldots, n \), where \( \alpha > \frac{1}{2} \) and \( \zeta > 0 \) is some constant, (4.1) holds with

\[
\| \Delta_1 \| \leq \frac{u_{i}^{(1)} b}{|u_{i} b|} \sqrt{\frac{1}{2\alpha - 1}},
\]

\[
\| \Delta_k \| \leq \frac{u_{i}^{(1)} b}{|u_{i} b|} \sqrt{\frac{k^2}{(2\alpha + 1)(2\alpha - 1)} + \frac{k - 1}{2\alpha - 1} |L_{2i}^{(k)}(0)|}, \quad k = 2, \ldots, k_0,
\]

\[
\| \Delta_k \| \leq \sqrt{\frac{k^2}{4\alpha^2 - 1} + \frac{k - 1}{2\alpha - 1} |L_{2i}^{(k)}(0)|}, \quad k = k_0 + 1, \ldots, n - 1.
\]
Proof. Notice that $|\Delta_k| \leq |L_k^{(k)}(0)||\tilde{\Delta}_k|$ still holds with $\tilde{\Delta}_k$ defined by (4.13). We only need to accurately bound the right-hand side of (4.14). For $k = 1, 2, \ldots, n - 1$, from (4.17) we obtain

$$
\left( \sum_{j=k+1}^{n} \frac{\sigma_j^2 |u_j^T b|^2}{\sigma_j} \right)^{1/2} = \sigma_{k+1} |u_{k+1}^T b| \left( \sum_{j=k+1}^{n} \frac{\sigma_j^2 |u_j^T b|^2}{\sigma_{k+1}^2 |u_{k+1}^T b|^2} \right)^{1/2} \\
\leq \sigma_{k+1} |u_{k+1}^T b| \left( \sum_{j=k+1}^{n} \frac{\sigma_j^2}{\sigma_{k+1}} \right)^{1/2} \\
= \sigma_{k+1} |u_{k+1}^T b| \left( \sum_{j=k+1}^{n} \left( \frac{j}{k+1} \right)^{-2\alpha} \right)^{1/2} \\
= \sigma_{k+1} |u_{k+1}^T b| \left( (k+1)^{2\alpha} \sum_{j=k+1}^{n} \frac{1}{j^{2\alpha}} \right)^{1/2} \\
< \sigma_{k+1} |u_{k+1}^T b|(k+1)^{\alpha} \left( \int_{k}^{\infty} \frac{1}{x^{2\alpha}} dx \right)^{1/2} \\
= \sigma_{k+1} |u_{k+1}^T b| \left( \frac{k+1}{k} \right)^{\alpha} \sqrt{\frac{k}{2\alpha - 1}} \\
= \sigma_{k+1} |u_{k+1}^T b| \frac{\sigma_k}{\sigma_{k+1}} \sqrt{\frac{k}{2\alpha - 1}} \\
= \sigma_k |u_{k+1}^T b| \sqrt{\frac{k}{2\alpha - 1}}.
$$

(4.28)

Since the function $x^{2\alpha}$ with any $\alpha > \frac{1}{2}$ is convex over the interval $[0, 1]$, for $k = 2, \ldots, k_0$, from (4.15) we obtain

$$
\left( \sum_{j=1}^{k} \frac{1}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2} = \frac{1}{\sigma_k |u_k^T b|} \left( \sum_{j=1}^{k} \frac{\sigma_j^2 |u_j^T b|^2}{\sigma_k^2 |u_k^T b|^2} \right)^{1/2} \\
= \frac{1}{\sigma_k |u_k^T b|} \left( \sum_{j=1}^{k} \left( \frac{j}{k} \right)^{2\alpha(1+\beta)} \right)^{1/2} \\
= \frac{1}{\sigma_k |u_k^T b|} \left( k \sum_{j=1}^{k} \left( \frac{j-1}{k} \right)^{2\alpha(1+\beta)} + 1 \right)^{1/2} \\
< \frac{1}{\sigma_k |u_k^T b|} \left( k \int_{0}^{1} x^{2\alpha(1+\beta)} dx + 1 \right)^{1/2} \\
= \frac{1}{\sigma_k |u_k^T b|} \sqrt{\frac{k}{2\alpha(1+\beta) + 1}} + 1.
$$

(4.29)

Substituting the above and (4.28) into (4.14) yields (4.26). For $k = 1$, (4.25) follows
from (4.19). For $k = k_0 + 1, \ldots, n - 1$, from (4.15) and (4.16), by (4.29) we obtain
\[
\left( \sum_{j=1}^{k} \frac{1}{\sigma_j^2 |u_j^2 b|^2} \right)^{1/2} \leq \sum_{j=1}^{k} \frac{\sigma^2_j u_j^2 b^2}{\sigma_j^2 |u_j^2 b|^2} \leq \sum_{j=1}^{k} \frac{\sigma^2_j}{\sigma_j^2} \leq \frac{1}{\sigma_k |u_k b|} \sqrt{\frac{k}{2\alpha + 1} + 1}.
\]
Combining it with (4.28) yields (4.27).

For moderately and mildly ill-posed problems, it turns out impossible to estimate $|L_j^{(k)}(0)|, j = 1, 2, \ldots, k$ both elegantly and accurately unless $\alpha > 1$ sufficiently.

**Theorem 4.4.** For a moderately and mildly ill-posed problem with $\sigma_i = \zeta i^{-\alpha}, i = 1, 2, \ldots, n$ and suitable $\alpha > 1$, for $k = 2, 3, \ldots, n - 1$ we have

\[
|L_j^{(k)}(0)| \approx \left( 1 + \frac{j}{2\alpha + 1} \right) \prod_{i=j+1}^{k} \left( \frac{j}{i} \right)^{2\alpha}, \quad j = 1, 2, \ldots, k - 1,
\]

\[
\frac{k}{2\alpha + 1} \leq |L_{k_1}^{(k)}(0)| \approx 1 + \frac{k}{2\alpha + 1}
\]

with the lower bound requiring that $k$ satisfy $\frac{2\alpha + 1}{k} \leq 1$; for $\frac{1}{2} < \alpha \leq 1$ and $k$ satisfying $\frac{2\alpha + 1}{k} \leq 1$, we have

\[
\frac{k}{2\alpha + 1} < |L_{k_1}^{(k)}(0)|.
\]

**Proof.** Exploiting the first order Taylor expansion, we obtain estimate
\[
|L_j^{(k)}(0)| = \prod_{i=1}^{k-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} = \prod_{i=1}^{k-1} \frac{1}{1 - \left( \frac{i}{k} \right)^{2\alpha}}
\]
\[
\approx 1 + \sum_{i=1}^{k-1} \left( \frac{i}{k} \right)^{2\alpha} = 1 + k \sum_{i=1}^{k} \frac{1}{k} \left( \frac{i-1}{k} \right)^{2\alpha}
\]
\[
\approx 1 + k \int_0^1 x^{2\alpha} dx = 1 + \frac{k}{2\alpha + 1}.
\]

For $j = 1, 2, \ldots, k - 1$, by the definition of $\sigma_i$, since $\alpha \geq \frac{1}{2}$, we have

\[
|L_j^{(k)}(0)| = \prod_{i=1, i \neq j}^{k} \left| \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} \right| = \prod_{i=1}^{j-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} \cdot \prod_{i=j+1}^{k} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2}
\]
\[
= \prod_{i=1}^{j-1} \frac{1}{1 - \left( \frac{i}{j} \right)^{2\alpha}} \prod_{i=j+1}^{k} \frac{1}{1 - \left( \frac{i}{j} \right)^{2\alpha}}
\]
\[
\approx \left( 1 + \sum_{i=1}^{j-1} \left( \frac{i}{j} \right)^{2\alpha} \right) \left( 1 + \sum_{i=j+1}^{k} \left( \frac{i}{j} \right)^{2\alpha} \right) \prod_{i=j+1}^{k} \left( \frac{j}{i} \right)^{2\alpha}
\]
\[
\leq \left( 1 + \int_0^1 x^{2\alpha} dx \right) \left( 1 + j^{2\alpha} \int_j^k \frac{1}{x^{2\alpha}} dx \right) \prod_{i=j+1}^{k} \left( \frac{j}{i} \right)^{2\alpha}
\]
\[
= \left( 1 + \frac{j}{2\alpha + 1} \right) \left( 1 + \frac{j - 2\alpha k - 2\alpha + 1}{2\alpha - 1} \right) \prod_{i=j+1}^{k} \left( \frac{j}{i} \right)^{2\alpha}.
\]
Note that $\prod_{i=j+1}^{k} \left( \frac{j}{k} \right)^{2\alpha}$ are always smaller than one for $j = 1, 2, \ldots, k - 1$, and the smaller $j$ is, the smaller it is. Furthermore, exploiting
\[\left( \frac{j}{k} \right)^{k-j} < \prod_{i=j+1}^{k} \frac{j}{i} < \left( \frac{j}{j+1} \right)^{k-j},\]
by some elementary manipulation, for suitable $\alpha > 1$ we can justify the estimates
\[\frac{j - j^{2\alpha} k^{2\alpha+1}}{2\alpha - 1} \prod_{i=j+1}^{k} \left( \frac{j}{i} \right)^{2\alpha} \approx 0, \quad j = 1, 2, \ldots, k - 1.\]
As a result, for suitable $\alpha > 1$ we have
\[|L_j^{(k)}(0)| \approx \left( 1 + \frac{j}{2\alpha + 1} \right) \prod_{i=j+1}^{k} \left( \frac{j}{i} \right)^{2\alpha}, \quad j = 1, 2, \ldots, k - 1,\]
which proves (4.31). The right-hand side of (4.32) follows from the monotonic increasing property of the right-hand side of (4.31) with respect to $j$.

On the other hand, once $k$ is such that $\frac{2\alpha+1}{k} \leq 1$, we always have
\[|L_{k_1}^{(k)}(0)| \geq |L_k^{(k)}(0)| = \prod_{i=1}^{k-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_k^2} = \prod_{i=1}^{k-1} \frac{1}{1 - \left( \frac{k}{i} \right)^{2\alpha}} > 1 + \sum_{i=1}^{k-1} \left( \frac{i}{k} \right)^{2\alpha} > 1 + k \int_{0}^{\frac{1}{k}} x^{2\alpha} dx = 1 + \frac{k}{2\alpha + 1} \approx 1 + \frac{k}{2\alpha + 1} \left( 1 - \frac{2\alpha + 1}{k} \right) = \frac{k}{2\alpha + 1},\]
which yields the lower bound of (4.32) and (4.33).

**Remark 4.4.** The inaccuracy source of (4.34) and (4.31) consists in using the summation $\Sigma$ to replace the product $\Pi$ approximately in the proof. They are considerable underestimates for $\frac{1}{2} < \alpha \leq 1$ but are accurate for suitable $\alpha > 1$; the bigger $\alpha$ is, the more accurate the estimates (4.34) and (4.31) are. The derivation of (4.35) indicates that $|L_{k_1}^{(k)}(0)|$ can be substantially bigger than $\frac{k}{2\alpha + 1}$ for $\frac{1}{2} < \alpha \leq 1$, particularly when $\alpha$ is close to $\frac{1}{2}$; in this case, $|L_{k_1}^{(k)}(0)|$ cannot be bounded from above.

**Remark 4.5.** (4.31) shows that the first two points in Remark 4.3 are still true.

**Remark 4.6.** For severely ill-posed problems, under assumptions (4.15)–(4.17), we have $\frac{\sigma_{i+1}}{\sigma_k} \sim \rho^{-1}$, $\frac{|u_{i+1}^R|}{|u_k^R|} \sim \rho^{-1-\beta} < 1$ for $k \leq k_0$ and $\frac{|u_{i+1}^R|}{|u_k^R|} = 1$ for $k > k_0$. Therefore, from (4.24), we see that $\| \sin(\mathcal{V}_k, \mathcal{V}_k^R) \|$ do not exhibit either increasing or decreasing tendency for $k = 1, 2, \ldots, k_0$ and $k = k_0 + 1, \ldots, n - 1$, respectively, as is numerically justified by Figure 1 (c). However, the situation is different for moderately ill-posed problems. For them, notice that $\frac{|u_{i+1}^R|}{|u_k^R|} = \left( \frac{k}{k+1} \right)^{\alpha(1+\beta)}$ increases slowly and approaches one with $k$ increasing to $k_0$ and $\frac{|u_{i+1}^R|}{|u_k^R|} = 1$ for $k > k_0$, and $\sqrt{\frac{k^2}{2\alpha - 1}} |L_{k_1}^{(k)}(0)|$ increases as $k$ grows. Therefore, (4.27) illustrates that $\| \sin(\mathcal{V}_k, \mathcal{V}_k^R) \|$ exhibits increasing tendency with $k$. This means that $\mathcal{V}_k^R$ may not
capture $V_k$ so well as it does for severely ill-posed problems as $k$ increases. In particular, $\| \sin \Theta(V_k, V_k^R) \|$ starts to approach one as $k$ increases up to some point, meaning that $V_k^R$ will contain substantial information on the right singular vectors corresponding to the $n-k$ small singular values of $A$.

Remark 4.7. Regarding mildly ill-posed problems, for the same noise level $\| e \|$ and $\beta$, firstly, the factor $\frac{u_{k+1}^T u_k}{u_k^T u_k} = \left( \frac{k}{k+1} \right)^{\alpha(1+\beta)}$ is bigger than that for a moderately ill-posed problem for the same $k \leq k_0$; secondly, (4.35) and the comment on it indicate that $|L_{k_1}^{(k)}(0)|$ is substantially bigger than one for $\frac{1}{2} < \alpha \leq 1$. The bound (4.27) thus becomes increasingly large as $k$ increases, causing that $\| \Delta_k \|$ is large and $\| \sin \Theta(V_k, V_k^R) \| \approx 1$ soon. Consequently, as $k$ increases, $V_k^R$ cannot effectively capture $V_k$ and contains substantial information on the right singular vectors corresponding to the $n-k$ small singular values.

Taking the moderately ill-posed heat of $n = 1024$ from [34], we now illustrate the sharpness of (4.1) when inserting the estimates (4.25)–(4.26) into it, where we take the equalities in (4.25) and (4.26) with $\beta = 0$ and $|L_{k_1}^{(k)}(0)| = 1 + \frac{1}{k_{\alpha} - 1}$ from (4.32). Regarding the determination of $\alpha$, Figure 2 (a) draws the first 400 singular values of heat and model singular values $\sigma_i = \frac{1}{k_i}$, from which we see that the first 150 model singular values decay faster than those of heat and the rest ones decay more slowly than those of heat. As a result, we take $\alpha = 3$ as a rough estimate, and use it in our above estimates.

For heat, Figure 2 (b) plots $|L_{j}^{(k)}(0)|$, $j = 1, 2, \ldots, k$ computed by the formula (4.4) for $k = 2, 3, \ldots, 20$. As we can see, the behavior of $|L_j^{(k)}(0)|$ is similar to that for the severely ill-posed problem shaw. The difference is that $|L_{k_1}^{(k)}(0)|$ now increases slowly with $k$ and $\max_{k=2,3,\ldots,20} |L_{k_1}^{(k)}(0)| \approx 49.6230$, considerably bigger than one. Figure 2 (c) shows that our estimates for $\| \sin \Theta(V_k, V_k^R) \|$ match the exact ones quite well for $k = 1, 2, \ldots, 25$. We have found that the maximum and minimum of these ratios are 1.4612 and 0.9487, respectively, and the geometrical mean of the ratios is 1.0791. More precisely, the fifteen ratios are 1.2130, 1.3429, 1.0899, 1.4499, 1.0222, 1.0556, 1.0023, 0.9487, 0.9603, 1.4612, 1.0067, 1.0037, 1.0079, 1.0025, 0.9962, 1.0186, 1.4264, 1.0000, 1.0023, 1.0034, 1.0039, 1.0140, 1.1938, 1.0000, 1.0004, respectively. All these results indicate that our estimates for $\| \sin \Theta(V_k, V_k^R) \|$ are sharp and realistic. We also plot the semi-convergence process of LSQR and the TSVD method; see Figure 2 (d), where the transition point $k_0 = 33$ of the TSVD method but the semi-convergence of LSQR occurs at $k^* = 23$, considerably smaller than $k_0$. Based on Theorem 3.1, this implies that the $k$ Ritz values $\theta_i^{(k)}$ must not approximate the large singular values of $A$ in natural order for some $k \leq k^*$. We have numerically confirmed this by comparing the $\theta_i^{(k)}$ and the first $k+1$ singular values $\sigma_i$ for $k \leq k^*$. We will report the details in the next section.

We now numerically justify our results by using a random mildly ill-posed problem regutm [34] with the prescribed singular values $\sigma_i = i^{-0.6}$ and the random left and right singular vectors $u_i$, $v_i$, $i = 1, 2, \ldots, n$ having exactly $i-1$ sign changes. We take $m = n = 10^4$, set $x_{true} = ones(n, 1)$, and generate $b_{true} = Ax_{true}$. Then we generate the noisy $b = b_{true} + e$ with the relative noise level $\varepsilon = 10^{-3}$.

For regutm, Figure 3 (a) depicts the exact and estimated $\| \sin \Theta(V_k, V_k^R) \|$ for $k = 1, 2, \ldots, 10$. Unlike what we have done on shaw and heat, since $\alpha = 0.6$, it is known from Theorem 4.4 that $|L_{k_1}^{(k)}(0)|$ cannot bounded from above. Therefore, we compute $|L_{k_1}^{(k)}(0)|$ by its definition directly, and find $\max_{k=2,3,\ldots,10} |L_{k_1}^{(k)}(0)| \approx 3963,$
The indices $k$ of singular values $10^{-12}$ $10^{-10}$ $10^{-8}$ $10^{-6}$ $10^{-4}$ $10^{-2}$ $10^0$ $10^2$ $10^4$ $10^6$ $10^8$ $10^{10}$

Singular values $\sigma_1 = \frac{1}{2}$; (b): plots of $|L_j^{(k)}(0)|$ for $k = 1, 2, \ldots, 20$; (c): the exact and estimated $\|\sin(\Theta(V_k, V_R^k))\|$; (d): the semi-convergence process of LSQR and TSVD.

substantially bigger than those for shaw and heat. Figure 3 (a) depicts the exact $\|\sin(\Theta(V_k, V_R^k))\|$ and the estimates for them. We find that the maximum and minimum of the exact and estimated ones are 1 and 0.6217, and the geometric mean of the ten ratios is 0.9060. Precisely, the ten ratios are $0.6217, 0.7763, 0.8492, 0.9272, 0.9820, 0.9993, 0.9999, 0.9999, 1.0000, 1.0000$, respectively. The exact and estimated $\|\sin(\Theta(V_k, V_R^k))\|$ approach one quickly as $k$ increases. Figure 3 (b) illustrates that $|L_j^{(k)}(0)|$ increases faster with $k$ than that in heat and $|L_j^{(k)}(0)|$ for a fixed $k$ and exhibits increasing tendency with respect to $j$ until $j$ is close to $k$ but not equal to $k$.

For $k = 2, 3, \ldots, 10$, Figure 4 plots $|L_j^{(k)}(0)|$ when taking the model singular values $\sigma_i = \frac{1}{\alpha^i}$ with $\alpha = 1$ and 4. Combining Figure 2 (b) for heat, Figure 3 (b) for regutm and the observations on them, we find from Figure 4 that (i) the smaller $\alpha$ is, the bigger $|L_j^{(k)}(0)|$ is for the same $k$ and (ii) the bigger $\alpha$ is, the smaller $|L_j^{(k)}(0)|$ is
for a fixed k and the same small j. Together with Figure 3 (b) for regutm, we find that, for k = 10, \( |L_{k_1}^{(k)}(0)| \approx 3962.7 \) for \( \alpha = 0.6 \), \( |L_{k_1}^{(k)}(0)| \approx 199.88 \) for \( \alpha = 1 \), and \( |L_{k_1}^{(k)}(0)| \approx 2.2877 \) for \( \alpha = 4 \). We have also found that \( |L_{k_1}^{(k)}(0)| \approx 3.5103 \) for \( \alpha = 3 \) when \( k = 10 \). Actually, the two estimates are 2.4286 and 2.1111 for \( \alpha = 3 \) and 4, respectively. Therefore, \( 1 + \frac{k}{2\alpha + 1} \) is indeed a good estimate for \( |L_{k_1}^{(k)}(0)| \) for suitable \( \alpha > 1 \). Moreover, the bigger \( \alpha \), the more accurate \( 1 + \frac{k}{2\alpha + 1} \) is as an estimate for \( |L_{k_1}^{(k)}(0)| \). On the other hand, if \( \alpha \) is small, e.g., \( \alpha = 0.6 \) and \( 1 + \frac{k}{2\alpha + 1} \) underestimates \( |L_{k_1}^{(k)}(0)| \) very considerably. For \( k = 2, 3, \ldots, 10 \), we also observe that \( |L_{k_1}^{(k)}(0)| > \frac{k}{2\alpha + 1} \) always holds, which confirms the low bounds in (4.32) and (4.33).

![Fig. 4. Plots of \( |L_{j}^{(k)}(0)| \) for the model singular values \( \sigma_i = \frac{1}{\sqrt{i}} \) with \( \alpha = 1 \) and \( \alpha = 4 \).](image)

5. A manifestation of \( \sin \Theta \) theorems on the behavior of Ritz values \( \theta_k^{(k)} \).

In this section, we investigate how \( \| \sin \Theta(V_k, V_k^R) \| \) affects the smallest Ritz value \( \theta_k^{(k)} \).

We aim at achieving a manifestation that (i) we may have \( \theta_k^{(k)} > \sigma_{k+1} \), that is, no small Ritz value may appear for suitable \( \| \sin \Theta(V_k, V_k^R) \| < 1 \), and (ii) we must have \( \theta_k^{(k)} < \sigma_{k+1} \), that is, the k Ritz values \( \theta_k^{(k)} \) do not approximate the large singular values of \( A \) in natural order, when \( \| \sin \Theta(V_k, V_k^R) \| \) is sufficiently close to one.

**Theorem 5.1.** Let \( \| \sin \Theta(V_k, V_k^R) \|^2 = 1 - \varepsilon_k^2 \) with \( 0 < \varepsilon_k < 1 \), \( k = 1, 2, \ldots, n - 1 \), and let the unit-length \( \tilde{q}_k \in V_k^R \) be the vector that has the smallest angle with \( V_k^\perp \), i.e., the closest to \( V_k^\perp \), where \( V_k^\perp \) is the matrix consisting of the last \( n - k \) columns of \( V \) defined by (1.5). Then it holds that

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

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

\[
\sqrt{\tilde{q}_k^T A^T A \tilde{q}_k} > \sigma_{k+1};
\]

if \( \varepsilon_k^2 \leq \frac{\delta}{\sigma_{k+1}} \) 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., \( \| \sin \Theta(V_k, V_k^R) \| \) is sufficiently close to one.
Proof. Since the columns of $Q_k$ generated by Lanczos bidiagonalization form an orthonormal basis of $V_k^R$, by definition and the assumption on $\hat{q}_k$ we have

$$
\|\sin(\Theta(V_k, V_k^R))\| = \|(V_k^\perp)\q{T}Q_k\| = \max_{\|c\|=1} \|V_k^\perp(V_k^\perp)\q{T}Q_k c\| = \|V_k^\perp(V_k^\perp)\q{T}Q_k c_k\|
$$

(5.4)

with $\hat{q}_k = Q_k c_k \in V_k^R$ and $\|c_k\| = 1$.

Expand $\hat{q}_k$ as the following orthogonal direct sum decomposition:

$$
\hat{q}_k = V_k^\perp(V_k^\perp)^T \hat{q}_k + V_k V_k^T \hat{q}_k.
$$

(5.5)

Then from $\|\hat{q}_k\| = 1$ and (5.4) we obtain

$$
\|V_k^T \hat{q}_k\| = \|V_k V_k^T \hat{q}_k\| = \sqrt{1 - \|V_k^\perp(V_k^\perp)^T \hat{q}_k\|^2} = \sqrt{1 - (1 - \varepsilon_k^2)} = \varepsilon_k.
$$

(5.6)

From (5.5), we next bound the Rayleigh quotient of $\hat{q}_k$ with respect to $A^T A$ from below. By the SVD (1.5) of $A$ and $V = (V_k, V_k^\perp)$, we partition

$$
\Sigma = \begin{pmatrix}
\Sigma_k & \Sigma_k^\perp \\
\Sigma_k^\perp & \Sigma_k
\end{pmatrix},
$$

where $\Sigma_k = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_k)$ and $\Sigma_k^\perp = \text{diag}(\sigma_{k+1}, \sigma_{k+2}, \ldots, \sigma_n)$. Making use of $A^T A V_k = V_k \Sigma_k^2$ and $A^T A V_k^\perp = V_k^\perp (\Sigma_k^2)^2$ as well as $V_k^T V_k^\perp = 0$, we obtain

$$
\hat{q}_k^T A^T A \hat{q}_k = (V_k^\perp(V_k^\perp)^T \hat{q}_k + V_k V_k^T \hat{q}_k)^T A^T A (V_k^\perp(V_k^\perp)^T \hat{q}_k + V_k V_k^T \hat{q}_k)
$$

$$
= (\hat{q}_k^T V_k^\perp(V_k^\perp)^T \hat{q}_k + \hat{q}_k^T V_k V_k^T) (V_k^\perp(\Sigma_k^2)^2(V_k^\perp)^T \hat{q}_k + V_k \Sigma_k^2 V_k^T \hat{q}_k)
$$

(5.7)

$$
= \hat{q}_k^T V_k^\perp (\Sigma_k^2)^2(V_k^\perp)^T \hat{q}_k + \hat{q}_k^T V_k \Sigma_k^2 V_k^T \hat{q}_k.
$$

$(V_k^\perp)^T \hat{q}_k$ and $V_k^T \hat{q}_k$ are unlikely to be the eigenvectors of $(\Sigma_k^2)^2$ and $\Sigma_k^2$ associated with their respective smallest eigenvalues $\sigma_n^2$ and $\sigma_k^2$ simultaneously, which are the $(n - k)$-th canonical vector $e_{n - k}^{(k)}$ of $\mathbb{R}^{n - k}$ and the $k$-th canonical vector $e_k^{(k)}$ of $\mathbb{R}^k$, respectively; otherwise, $\hat{q}_k = v_n$ and $\hat{q}_k = v_k$ simultaneously, which are impossible as $k < n$. Therefore, from (5.7), (5.4) and (5.6), we obtain the strict inequality

$$
\hat{q}_k^T A^T A \hat{q}_k > \|(V_k^\perp)^T \hat{q}_k\|^2 \sigma_n^2 + \|V_k^T \hat{q}_k\|^2 \sigma_k^2 = (1 - \varepsilon_k^2)\sigma_n^2 + \varepsilon_k^2 \sigma_k^2,
$$

from which it follows that the lower bound of (5.1) holds. By a similar argument, from (5.7) and (5.4), (5.6) we obtain the upper bound of (5.1):

$$
\hat{q}_k^T A^T A \hat{q}_k < \|(V_k^\perp)^T \hat{q}_k\|^2 (\Sigma_k^2)^2 + \|V_k^T \hat{q}_k\|^2 \Sigma_k^2 = (1 - \varepsilon_k^2)\sigma_k^2 + \varepsilon_k^2 \sigma_k^2.
$$

From the lower bound of (5.1), 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 $\hat{q}_k^T A^T A \hat{q}_k > \sigma_{k+1}$, i.e., (5.2) holds.

From (2.4), we obtain $B_k^T B_k Q_k = Q_k^T A^T A Q_k$. Note that $(\theta_k^{(k)})^2$ is the smallest eigenvalue of the symmetric positive definite matrix $B_k^T B_k$. Therefore, we have

$$
(\theta_k^{(k)})^2 = \min_{\|c\|=1} c^T Q_k^T A^T A Q_k c = \min_{c \in V_k^R, \|c\|=1} c^T A^T A c = \hat{q}_k^T A^T A \hat{q}_k,
$$

(5.8)
where \( \hat{q}_k \) is, in fact, the Ritz vector of \( A^T A \) from \( V_k^R \) corresponding to the smallest Ritz value \( (\theta_k^{(k)})^2 \). Therefore, we have

\[
(5.9) \quad \theta_k^{(k)} \leq \sqrt{\hat{q}_k^T A^T A \hat{q}_k},
\]

from which it follows from (5.1) that \( (\theta_k^{(k)})^2 < (1 - \varepsilon_k^2) \sigma_k^2 + \varepsilon_k^2 \sigma_1^2 \). For any \( \delta > 0 \), we can choose \( \varepsilon_k \geq 0 \) such that

\[
(\theta_k^{(k)})^2 < (1 - \varepsilon_k^2) \sigma_k^2 + \varepsilon_k^2 \sigma_1^2 \leq (1 + \delta) \sigma_k^2,
\]

i.e., (5.3) holds, solving which for \( \varepsilon_k^2 \) gives \( \varepsilon_k^2 \leq \frac{\delta}{(\varepsilon_k^2+1)^2-1} \).

Since \( V_k \) is the orthogonal complement of \( \text{span}\{V_k^L\} \), by assumption, \( \hat{q}_k \in V_k^R \) has the largest acute angle with \( V_k \), that is, it is the vector in \( V_k^R \) that contains the least information on \( V_k \). On the other hand, in the sense of (5.8), \( \hat{q}_k \in V_k^R \) is the optimal vector that extracts the least information from \( V_k \) and the richest information from \( \text{span}\{V_k^L\} \). From Theorem 5.1, since \( V_k \) is the orthogonal complement of \( \text{span}\{V_k^L\} \), we know that \( \hat{q}_k \in V_k^R \) has the largest acute angle with \( V_k \), that is, it contains the least information from \( V_k \) and the richest information from \( \text{span}\{V_k^L\} \) in the sense of (5.8). Therefore, \( \hat{q}_k \) and \( \hat{q}_k \) have a similar optimality, and consequently

\[
(5.10) \quad \theta_k^{(k)} \approx \sqrt{\hat{q}_k^T A^T A \hat{q}_k}.
\]

Combining this estimate with (5.2) and (5.9), we may have \( \theta_k^{(k)} > \sigma_k+1 \) if \( \varepsilon_k \geq \frac{\sigma_k+1}{\sigma_k} \).

We analyze \( \theta_k^{(k)} \) and inspect the condition \( \varepsilon_k \geq \frac{\sigma_k+1}{\sigma_k} \) for (5.2) and get insight into if the true (or actual) \( \varepsilon_k \) resulting from the three kinds of ill-posed problems satisfies it. The condition \( \varepsilon_k \geq \frac{\sigma_k+1}{\sigma_k} \sim \rho^{-1} \) for severely ill-posed problems, meaning that \( \| \sin \Theta(V_k, V_k^R) \| \) is approximately smaller than \( 1 - \frac{1}{2} \rho^{-2} \). For moderately ill-posed problems with \( \alpha > 1 \), the lower bound \( \sigma_k+1/\sigma_k \) increases with \( k \leq k_0 \), and it cannot be close to one for suitable \( \alpha > 1 \); for mildly ill-posed problems with \( \alpha < 1 \), the lower bound for \( \varepsilon_k \) increases faster than it does for moderately ill-posed problems, and it may well approach one for \( k \) small. Therefore, the condition \( \varepsilon_k \geq \frac{\sigma_k+1}{\sigma_k} \) for (5.2) requires that \( \| \sin \Theta(V_k, V_k^R) \| \) be not close to one for severely and moderately ill-posed problems, but it must be fairly small for mildly ill-posed problems.

In view of (4.1) and \( \| \sin \Theta(V_k, V_k^R) \|^2 = 1 - \varepsilon_k^2 \), we have \( \| \Delta_k \|^2 = \frac{1-\varepsilon_k^2}{\varepsilon_k^2} \). Thus, the condition \( \varepsilon_k \geq \frac{\sigma_k+1}{\sigma_k} \) for (5.2) amounts to requiring that \( \| \Delta_k \| \) cannot be large for severely and moderately ill-posed problems but it must be fairly small for mildly ill-posed problems. Unfortunately, Theorems 4.1–4.3 and the remarks on them indicate that \( \| \Delta_k \| \) increases with \( k \) and is generally large for a mildly ill-posed problem, while \( \| \Delta_k \| \) is modest and increases slowly with \( k \) for a moderately ill-posed problem with suitable \( \alpha > 1 \), and, by (4.24), \( \| \Delta_k \| \) is approximately \( \rho^{-2+\beta} \), considerably smaller than one for a severely ill-posed problem with \( \rho > 1 \) not close to one. Consequently, for mildly ill-posed problems, the actual \( \| \Delta_k \| \) can hardly be small and is generally large, namely, the true \( \varepsilon_k \) is small, which causes that the condition \( \varepsilon_k \geq \frac{\sigma_k+1}{\sigma_k} \) fails to meet soon as \( k \) increases, while it is satisfied for severely or moderately ill-posed problems with suitable \( \rho > 1 \) or \( \alpha > 1 \).

Now let us report numerical experiments to confirm Theorem 5.1 and the above remarks. Besides the previous severely, moderately and mildly problems shaw, heat
and regutm, we also test the problem deriv2 of $n = 10^4$ from [34], in which we take the parameter “example = 7”. This continuous first kind Fredholm integral equation is mildly ill-posed [34] but the singular values $\sigma_i$ of the matrix deriv2 after discretization decay very like $\frac{1}{i}$ and $\frac{\sigma_n}{\sigma_1} = 1.2e + 8$, which resembles a moderately ill-posed problem with $\alpha = 2$. We omit the figure comparison.

For each of the four problems, we first investigate the true $\| \sin \Theta(V_k, V_k^R) \|$ and the required $\| \sin \Theta(V_k, V_k^R) \|$ that makes (5.2) hold, from which (5.9) and (5.10) it is known that $\theta(k) > \sigma_{k+1}$ may hold. We take $\varepsilon_k = \frac{2 + i}{\sigma_k}$ and compute $\| \sin \Theta(V_k, V_k^R) \| = \sqrt{1 - \varepsilon_k}$. We aim to check how the sufficient conditions are met for each problem and given $k$. We depict the true $\| \sin \Theta(V_k, V_k^R) \|$ versus the required ones in Figures 5–8 (a) and draw the comparison diagrams of $k$ Ritz values $\theta(k)$ and first $k + 1$ large singular values $\sigma_i$ of the test matrices for each $k$ in Figures 5–8 (a). In Figure 9, we depict the semi-convergence processes of LSQR and the TSVD method for deriv2 and regutm, where, for deriv2 with the relative noise level $\varepsilon = 10^{-3}$, we see that the transition point $k_0 = 51$ of the TSVD method and the semi-convergence point $k^* = 21$ of LSQR and, for regutm with $\varepsilon = 10^{-3}$, $k^* = 25$ and $k_0 = 1423$. For each of these two problems, we find that $k^* \ll k_0$ but the best regularized solutions by LSQR and TSVD essentially have the same accuracy.

Figure 5 (a) indicates that for shaw the required sufficient conditions are met in the first 20 iterations except for $k = 18$. Figures 6–8 (a) indicate that for heat, deriv2 and regutm the sufficient conditions on $\| \sin \Theta(V_k, V_k^R) \|$ are satisfied until $k = 3$, $k = 5$ and $k = 2$, respectively, after which the true $\| \sin \Theta(V_k, V_k^R) \|$ starts to increase and approaches one quickly. These results justify our theory that (i) the sufficient conditions are met more easily for severely ill-posed problems than for moderately and mildly ill-posed problems, (ii) the smaller $\alpha$ is, the more quickly they approach one as $k$ increases, and (iii) for the latter two kinds of problems the true $\| \sin \Theta(V_k, V_k^R) \|$ exhibit monotonically increasing tendency and approach one with $k$.

Next we numerically investigate the behavior of the smallest Ritz value $\theta(k)$ and verify close relationships between it and the sufficient condition on $\| \sin \Theta(V_k, V_k^R) \|$. For shaw, we see from Figure 5 (b) the all the $\theta(k)$ are above $\sigma_{k+1}$ for $k = 1, 2, \ldots, 20$, including $k = 18$ at which the sufficient condition fails to meet. This indicates that the sufficient condition is not necessary for ensuring $\theta(k) > \sigma_{k+1}$. Nonetheless, we should find from Figure 5 (a) that the required $\| \sin \Theta(V_k, V_k^R) \|$ is only slightly bigger than the true $\| \sin \Theta(V_k, V_k^R) \|$. The experiments on heat, deriv2 and regutm have fully justified our theory. For heat, Figure 6 (b) clearly shows that the first $k$ large singular values $\sigma_i$ of heat, which includes $\theta(k) > \sigma_{k+1}$, for $k = 1, 2, 3$, at which the required sufficient conditions are satisfied, and $\theta(k) < \sigma_{k+1}$. This example illustrates that the required sufficient condition is also necessary and tight, for if they are not met then we will have $\theta(k) < \sigma_{k+1}$.

The numerical results on deriv2 are very similar to those on heat. From Figure 7 (b), we see that $\theta(k) > \sigma_{k+1}$ until $k = 6$, after which the the required sufficient condition fails to fulfill and $\theta(k) < \sigma_{k+1}$ appears. Regarding the mildly ill-posed regutm, the sufficient conditions are satisfied only for $k = 1, 2$, as is seen from Figure 8 (a). The $k$ Ritz values $\theta(k)$ interlace the $k + 1$ large singular values $\sigma_i$ in natural order only for $k = 1, 2$, and afterwards $\theta(k) < \sigma_{k+1}$, as indicated clearly by Figure 8 (b). Again, this demonstrates that our sufficient condition is tight. Moreover, compared
with the previous problems, we find that, generally, the more slowly the singular values decay, the harder the sufficient condition is to fulfill, thus the sooner $\theta^{(k)}_k < \sigma_{k+1}$ appears.

![Graph](image1.png)

**Fig. 5.** (a): The true $\|\sin(\Theta(V_k, V_R^k))\|$ and the required sufficient conditions on them; (b): $k$ Ritz values and the first $k+1$ large singular values of shaw, $k = 1, 2, \ldots, 21.$

![Graph](image2.png)

**Fig. 6.** (a) The true $\|\sin(\Theta(V_k, V_R^k))\|$ and the required sufficient conditions on them; (b): $k$ Ritz values and the first $k+1$ large singular values of heat, $k = 1, 2, \ldots, 11.$

![Graph](image3.png)

**Fig. 7.** (a): The true $\|\sin(\Theta(V_k, V_R^k))\|$ and the required sufficient conditions on them; (b): $k$ Ritz values and the first $k+1$ large singular values of deriv2, $k = 1, 2, \ldots, 15.$

### 6. Conclusions

For a general large-scale (1.1), the Krylov iterative solvers LSQR and CGLS are most popularly used. They have general regularizing effects and exhibit semi-convergence. If the regularized solutions at semi-convergence are best possible, the methods have the full regularization. In this case, complicated hybrid variants are not necessary, and we simply stop the methods after a few iterations.
The number $k$ of iterations

![Graph](image1)

**Fig. 8.** (a): The true $\|\sin(\Theta_k, V^R_k)\|$ and the required sufficient conditions on them; (b): $k$ Ritz values and the first $k+1$ large singular values of $\text{regutm}$, $k = 1, 2, \ldots, 10$.

The semi-convergence process of LSQR and TSVD for $\text{regutm}$, $k = 1, 2, \ldots, 10$.

![Graph](image2)

**Fig. 9.** (a): The semi-convergence process of LSQR and TSVD for $\text{deriv2}$ of $n = 10,000$; (b): the semi-convergence process of LSQR and TSVD for $\text{regutm}$ of $n = 10,000$ with $\sigma_k = \frac{1}{k^{\frac{1}{2}}}$.

when semi-convergence is recognized, which, in principle, can be determined by a suitable parameter-choice method, such as the L-curve criterion and the discrepancy principle.

In the simple singular value case, as a fundamental step towards understanding the regularization of LSQR, CGME and LSMR, we have established the $\sin \Theta$ theorem for the 2-norm distance between the underlying $k$ dimensional Krylov subspace and the $k$ dimensional dominant right singular subspace and derived accurate estimates on the distances for the three kinds of ill-posed problems under simplifying assumptions on the actual decay of the singular values of $A$. We have given detailed analyses on the results obtained. Then we have initially manifested some intrinsic relationships between the smallest Ritz values $\theta_k^{(k)}$ and $\|\sin(\Theta_k, V^R_k)\|$. The results will provide absolutely necessary background and ingredients for studying the problems mentioned in the beginning of Section 4.

We have reported illuminating numerical examples to show that our estimates are sharp and realistic, and have justified that our sufficient conditions on $\theta_k^{(k)} > \sigma_k + 1$ are tight and realistic. Also, we have numerically confirmed some other important properties on $|L_j^{(k)}(0)|$, $j = 1, 2, \ldots, k$.

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