# The regularization theory of the Krylov iterative solvers LSQR and CGLS for linear discrete ill-posed problems, part I: the simple singular value case

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**Abstract** For the large-scale linear discrete ill-posed problem min ||Ax - b|| or Ax = bwith b contaminated by a white noise, the Lanczos bidiagonalization based LSQR method and its mathematically equivalent Conjugate Gradient (CG) method for  $A^TAx =$  $A^Tb$  are most commonly used. They have intrinsic regularizing effects, where the number k of iterations plays the role of regularization parameter. However, there has been no answer to the long-standing fundamental concern by Björck and Eldén in 1979: for which kinds of problems LSQR and CGLS can find best possible regularized solutions? Here a best possible regularized solution means that it is at least as accurate as the best regularized solution obtained by the truncated singular value decomposition (TSVD) method or standard-form Tikhonov regularization. In this paper, assuming that the singular values of A are simple, we analyze the regularization of LSQR for severely, moderately and mildly ill-posed problems. We establish accurate estimates for the 2-norm distance between the underlying k-dimensional Krylov subspace and the k-dimensional dominant right singular subspace of A. For the first two kinds of problems, we then prove that LSQR finds a best possible regularized solution at semi-convergence occurring at iteration  $k_0$  and that, for  $k = 1, 2, \dots, k_0$ , (i) the k-step Lanczos bidiagonalization always generates a near best rank k approximation to A; (ii) the k Ritz values always approximate the first k large singular values in natural order; (iii) the k-step LSQR always captures the k dominant SVD components of A. For the third kind of problem, we prove that LSQR generally cannot find a best possible regularized solution. We derive estimates for the entries of the bidiagonal matrices generated by Lanczos bidiagonalization, which can be practically exploited to identify if LSQR finds a best possible regularized solution at semi-convergence. Numerical experiments confirm our theory.

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#### 1 Introduction and Preliminaries

Consider the linear discrete ill-posed problem

$$\min_{x \in \mathbb{R}^n} ||Ax - b|| \text{ or } Ax = b, \ A \in \mathbb{R}^{m \times n}, \ b \in \mathbb{R}^m,$$
 (1)

where the norm  $\|\cdot\|$  is the 2-norm of a vector or matrix, and A is extremely ill conditioned with its singular values decaying to zero without a noticeable gap. (1) mainly arises from the discretization of the first kind Fredholm integral equation

$$Kx = (Kx)(t) = \int_{\Omega} k(s,t)x(t)dt = g(s) = g, \ s \in \Omega \subset \mathbb{R}^q, \tag{2}$$

where the kernel  $k(s,t) \in L^2(\Omega \times \Omega)$  and g(s) are known functions, while x(t) is the unknown function to be sought. If k(s,t) is non-degenerate and g(s) satisfies the Picard condition, there exists the unique squares integrable solution x(t); see [23,44,47,69,76]. 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., [1,22,23,47,57,63,64,69,76,77,104]. The theory and numerical treatments of integral equations can be found in [69,70]. The right-hand side  $b = \hat{b} + e$  is noisy and assumed to be contaminated by a white noise e, caused by measurement, modeling or discretization errors, where  $\hat{b}$  is noise-free and  $\|e\| < \|\hat{b}\|$ . Because of the presence of noise e and the extreme ill-conditioning of e, the naive solution e0 to the true solution e1 to the true solution e1, where e2 denotes the Moore-Penrose inverse of a matrix. Therefore, one has to use regularization to extract a best possible approximation to e1.

In principle, regularizing an ill-posed problem is to replace it by a well-posed one, such that the error is compensated by the gain in stability. In other words, regularization is to compromise the error and stability as best as possible. For a white noise e, throughout the paper, we always assume that  $\hat{b}$  satisfies the discrete Picard condition  $\|A^{\dagger}\hat{b}\| \leq C$  with some constant C for n arbitrarily large [1,27,41,42,44,47,64]. It is an analog of the Picard condition in the finite dimensional case; see, e.g., [41], [44, p.9], [47, p.12] and [64, p.63]. The two dominating regularization approaches are to solve the following two essentially equivalent problems

$$\min_{x \in \mathbb{R}^n} ||Lx|| \text{ subject to } ||Ax - b|| = \min$$
 (3)

and general-form Tikhonov regularization (cf. [88,97,98])

$$\min_{x \in \mathbb{R}^n} \{ \|Ax - b\|^2 + \lambda^2 \|Lx\|^2 \}$$
 (4)

with  $\lambda > 0$  the regularization parameter for regularized solutions [44,47]. A suitable choice of the matrix L is based on a-prior information on  $x_{true}$ , and typically L is either the identity matrix, a diagonal weighting matrix, or a  $p \times n$  discrete approximation of a first or second order derivative operator. Particularly, if L = I, the identity matrix, (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), (3) and (4) can be fully analyzed by the singular value decomposition (SVD) of A. Let

$$A = U \begin{pmatrix} \Sigma \\ \mathbf{0} \end{pmatrix} V^T \tag{5}$$

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,  $\Sigma=\mathrm{diag}(\sigma_1,\sigma_2,\ldots,\sigma_n)\in\mathbb{R}^{n\times n}$  with the singular values  $\sigma_1>\sigma_2>\cdots>\sigma_n>0$  assumed to be simple throughout the paper, and the superscript T denotes the transpose of a matrix or vector. Then

$$x_{naive} = \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i} v_i = \sum_{i=1}^{n} \frac{u_i^T \hat{b}}{\sigma_i} v_i + \sum_{i=1}^{n} \frac{u_i^T e}{\sigma_i} v_i = x_{true} + \sum_{i=1}^{n} \frac{u_i^T e}{\sigma_i} v_i$$
 (6)

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

The discrete Picard condition means that, on average, the Fourier coefficients  $|u_i^T \hat{b}|$  decay faster than  $\sigma_i$  and enables regularization to compute useful approximations to  $x_{true}$ , which results in the following popular model that is used throughout Hansen's books [44,47] and the current paper:

$$|u_i^T \hat{b}| = \sigma_i^{1+\beta}, \ \beta > 0, \ i = 1, 2, \dots, n,$$
 (7)

where  $\beta$  is a model parameter that controls the decay rates of  $|u_i^T\hat{b}|$ . Hansen [47, p.68] points out, "while this is a crude model, it reflects the overall behavior often found in real problems." One precise definition of the discrete Picard condition is  $|u_i^T\hat{b}| = \tau_i\sigma_i^{1+\zeta_i}$  with certain constants  $\tau_i \geq 0$ ,  $\zeta_i > 0$ , i = 1, 2, ..., n. We remark that once the  $\tau_i > 0$  and  $\zeta_i$  do not differ greatly, such discrete Picard condition does not affect our claims, rather it complicates derivations and forms of the results.

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  $\mathscr{E}(\|e\|^2) = m\eta^2$  and  $\mathscr{E}(|u_i^T e|) = \eta$ ,  $i = 1, 2, \ldots, n$ , and  $\|e\| \approx \sqrt{m}\eta$  and  $|u_i^T e| \approx \eta$ ,  $i = 1, 2, \ldots, n$ ; see, e.g., [44, p.70-1] and [47, p.41-2]. The noise e thus affects  $u_i^T b$ ,  $i = 1, 2, \ldots, n$ , more or less equally. With (7), relation (6) shows that for large singular values  $|u_i^T \hat{b}|/\sigma_i$  is dominant relative to  $|u_i^T e|/\sigma_i$ . Once  $|u_i^T \hat{b}| \leq |u_i^T e|$  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

$$|u_{k_0}^T b| \approx |u_{k_0}^T \hat{b}| > |u_{k_0}^T e| \approx \eta, \ |u_{k_0+1}^T b| \approx |u_{k_0+1}^T e| \approx \eta;$$
 (8)

see [47, p.42, 98] and a similar description [44, p.70-1]. The  $\sigma_k$  are then divided into the  $k_0$  large ones and the  $n - k_0$  small ones.

The truncated SVD (TSVD) method [41,44,47] deals with (3) by solving

$$\min \|x\| \text{ subject to } \|A_k x - b\| = \min, \ k = 1, 2, \dots, n,$$
 (9)

where  $A_k = U_k \Sigma_k V_k^T$  is the best rank approximation k to A with respect to the 2-norm with  $U_k = (u_1, \ldots, u_k)$ ,  $V_k = (v_1, \ldots, v_k)$  and  $\Sigma_k = \operatorname{diag}(\sigma_1, \ldots, \sigma_k)$ ; it holds that  $\|A - A_k\| = \sigma_{k+1}$  (cf. [10, p.12]). and  $x_k^{tsvd} = A_k^{\dagger}b$ , called the TSVD solution, solves (9). An crucial observation is that  $x_k^{tsvd}$  is the minimum-norm least squares solution to  $\min_{x \in \mathbb{R}^n} \|A_k x - b\|$  that perturbs A to  $A_k$  in (1), and we will frequently exploit this interpretation later.

Based on the above properties of the white noise e, it is known from [44, p.70-1] and [47, p.71,86-8,95] that the TSVD solutions

$$x_{k}^{tsvd} = A_{k}^{\dagger}b = \begin{cases} \sum_{i=1}^{k} \frac{u_{i}^{T}b}{\sigma_{i}} v_{i} \approx \sum_{i=1}^{k} \frac{u_{i}^{T}\hat{b}}{\sigma_{i}} v_{i}, & k \leq k_{0}; \\ \sum_{i=1}^{k} \frac{u_{i}^{T}b}{\sigma_{i}} v_{i} \approx \sum_{i=1}^{k_{0}} \frac{u_{i}^{T}\hat{b}}{\sigma_{i}} v_{i} + \sum_{i=k_{0}+1}^{k} \frac{u_{i}^{T}e}{\sigma_{i}} v_{i}, & k > k_{0}, \end{cases}$$
(10)

and  $x_{k_0}^{tsvd}$  is the best TSVD regularized solution to (1), which balances the regularization and perturbation errors optimally and stabilizes the residual norms  $\|Ax_k^{tsvd} - b\|$  for k not close to n after  $k > k_0$ . The index k plays the role of the regularization parameter that determines how many large SVD components of A are used to compute a regularized solution  $x_k^{tsvd}$  to (1).

The solution  $x_{\lambda}$  of the Tikhonov regularization has a filtered SVD expansion

$$x_{\lambda} = \sum_{i=1}^{n} f_i \frac{u_i^T b}{\sigma_i} v_i, \tag{11}$$

where the  $f_i = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2}$  are called filters. The TSVD method is a special parameter filtered method, where, in  $x_k^{tsvd}$ , we take  $f_i = 1, i = 1, 2, ..., k$  and  $f_i = 0, i = k+1, ..., n$ . The error  $x_\lambda - x_{true}$  can be written as the sum of the regularization and perturbation errors, and an optimal  $\lambda_{opt}$  aims to balance these two errors and make the sum of their norms minimized [44,47,69,104]. The best possible regularized solution  $x_{\lambda_{opt}}$  retains the  $k_0$  dominant SVD components and dampens the other  $n-k_0$  small SVD components as much as possible [44,47]. Apparently, the ability to acquire *only* the largest SVD components of A is fundamental in solving (1).

A number of parameter-choice methods have been developed for finding  $\lambda_{opt}$  or  $k_0$ , such as the discrepancy principle [75], the L-curve criterion, whose use goes back to Miller [74] and Lawson and Hanson [72] and is termed much later and studied in detail in [43,49], and the generalized cross validation (GCV) [33,105]; see, e.g., [5, 44,47,64,66,68,79,89,104] for numerous comparisons. All parameter-choice methods aim to make  $f_i/\sigma_i$  not small for  $i=1,2,\ldots,k_0$  and  $f_i/\sigma_i\approx 0$  for  $i=k_0+1,\ldots,n$ . Each of these methods has its own merits and disadvantages, and no one is absolutely reliable for all ill-posed problems. For example, some of the mentioned parameter-choice methods may fail to find accurate approximations to  $\lambda_{opt}$ ; see [37,103] for an

analysis on the L-curve method and [44] for some other parameter-choice methods. A further investigation on paramater-choice methods is not our concern in this paper.

The TSVD method and the standard-form Tikhonov regularization produce very similar solutions with essentially the minimum 2-norm error, i.e., the worst-case error [69, p.13]; see [102], [42], [44, p.109-11] and [47, Sections 4.2 and 4.4]. Indeed, for an underlying linear compact equation Kx = g, e.g.,(2), with the noisy g and true solution  $x_{true}(t)$ , under the source condition that its solution  $x_{true}(t) \in \mathcal{R}(K^*)$  or  $x_{true}(t) \in \mathcal{R}(K^*K)$ , the range of the adjoint  $K^*$  of K or that of  $K^*K$ , which amounts to assuming that  $x_{true}(t)$  or its derivative is squares integrable, the errors of the best regularized solutions by the TSVD method and the Tikhonov regularization are *order optimal*, i.e., the same order as the worst-case error [69, p.13,18,20,32-40], [77, p.90] and [104, p.7-12]. These conclusions carries over to (1) [104, p.8]. Therefore, both  $x_{\lambda_{opt}}$  are best possible solutions to (1) under the above assumptions, and any of them can be taken as the reference standard when assessing the regularizing effects of an iterative solver. For the sake of clarity and analysis, we will take  $x_{k_0}^{tsvd}$  as the standard reference.

For (1) large, the TSVD method and the Tikhonov regularization method are generally too demanding, and only iterative regularization methods are computationally viable. A major class of methods has been Krylov iterative solvers that project (1) onto a sequence of low dimensional Krylov subspaces and computes iterates to approximate  $x_{true}$  [1,23,32,36,44,47,69]. Of Krylov iterative solvers, the CGLS (or CGNR) method, which implicitly applies the CG method [34,51] to  $A^TAx = A^Tb$ , and its mathematically equivalent LSQR algorithm [85] have been most commonly used. The Krylov solvers CGME (or CGNE) [10,11,19,36,38] and LSMR [11,25] are also choices, which amount to the CG method applied to min  $||AA^Ty - b||$  or  $AA^Ty = b$ with  $x = A^T y$  and MINRES [84] applied to  $A^T A x = A^T b$ , respectively. These Krylov solvers have been intensively studied and known to have general regularizing effects [1,21,32,36,38,44,47,52,53] and exhibit semi-convergence [77, p.89]; see also [10, p.314], [11, p.733], [44, p.135] and [47, p.110]: The iterates converge to  $x_{true}$  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  $x_{true}$  and instead converge to  $x_{naive}$ , 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 starts to inherit the ill-conditioning of (1) from some iteration onwards, and a small singular value of the projected problem amplifies the noise considerably.

The regularizing effects of CG type methods were noticed by Lanczos [71] and were rediscovered in [62,92,96]. Based on these works and motivated by a heuristic explanation on good numerical results with very few iterations using CGLS in [62], and realizing that such an excellent performance can only be expected if convergence to the regular part of the solution, i.e.,  $x_{k_0}^{tsvd}$ , takes place before the effects of ill-posedness show up, on page 13 of [12], Björck and Eldén in 1979 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 [44, p.145]. As remarked by Hanke and Hansen [39], the paper [12]

was the only extensive survey on algorithmic details until that time, and a strict proof of the regularizing properties of conjugate gradients is extremely difficult. An enormous effort has long been made to the study of regularizing effects of LSQR and CGLS (cf. [24,30,31,36,38,44,47,52,53,56,78,81,86,91,100]), but hitherto there has been no definitive answer to the above long-standing fundamental question, and the same is for CGME and LSMR.

For A symmetric, MINRES and MR-II applied to Ax = b directly are alternatives and have been shown to have regularizing effects [14,36,40,47,58,67], but MR-II seems preferable since the noisy b is excluded in the underlying subspace [55,58]. For A nonsymmetric or multiplication with  $A^T$  difficult to compute, GMRES and RRGMRES are candidate methods [3,15,16,80], and the latter may be better [58]. The hybrid approaches based on the Arnoldi process have been first proposed in [17] and studied in [14,18,73,82]. Gazzola and her coauthors [26,27,28,29] have described a general framework of the hybrid methods and presented various Krylov-Tikhonov methods with different parameter-choice strategies. The regularizing effects of these methods 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,  $V^TU$  is close to a diagonal matrix; for more details, see, e.g., [58] and [47, p.126].

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) was introduced in [54] and has been widely used [1,23,44,47,76]: If  $\sigma_j = \mathcal{O}(j^{-\alpha})$ , then (1) is mildly or moderately ill-posed for  $\frac{1}{2} < \alpha \le 1$  or  $\alpha > 1$ . If  $\sigma_j = \mathcal{O}(\rho^{-j})$  with  $\rho > 1$ ,  $j = 1,2,\ldots,n$ , then (1) is severely ill-posed. Here for mildly ill-posed problems we add the requirement  $\alpha > \frac{1}{2}$ , which does not appear in [54] but must be met for  $k(s,t) \in L^2(\Omega \times \Omega)$  in (1) [39,44]. In the one-dimensional case, i.e., q = 1, (1) is severely ill-posed with k(s,t) sufficiently smooth, and it is moderately ill-posed with  $\sigma_j = \mathcal{O}(j^{-p-1/2})$ , where p is the highest order of continuous derivatives of k(s,t); see, e.g., [44, p.8] and [47, p.10-11]. Clearly, the singular values  $\sigma_j$  for a severely ill-posed problem decay at the same rate  $\rho^{-1}$ , while those of a moderately or mildly ill-posed problem decay at the decreasing rate  $\left(\frac{j}{j+1}\right)^{\alpha}$  that approaches one more quickly with j for the mildly ill-posed problem than for the moderately ill-posed problem.

If a regularized solution to (1) is at least as accurate as  $x_{k_0}^{tsvd}$ , then it is called a best possible regularized solution. Given (1), if the regularized solution of an iterative regularization solver at semi-convergence is such a best possible one, then, by the words of Björck and Eldén, the solver *works* for the problem and is said to have the *full* regularization. Otherwise, the solver is said to have only the *partial* regularization.

Because it has long been unknown whether or not LSQR, CGLS, LSMR and CGME have the full regularization for a given (1), one commonly combines them with some explicit regularization, hoping that the resulting hybrid variants find best possible regularized solutions [1,44,47]. A hybrid CGLS is to run CGLS for several trial regularization parameters  $\lambda$  and picks up the best one among the candidates [1]. Its disadvantages are that regularized solutions cannot be updated with different  $\lambda$  and there is no guarantee that the selected regularized solution is a best possible one. The hybrid LSQR variants have been advocated by Björck and Eldén [12] and O'Leary and Simmons [83], and improved and developed by Björck [9] and Björck, Grimme

and van Dooren [13]. 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 the  $k_0$  dominant SVD components of A [9,13,39,83]. The explicit regularization for projected problems should be introduced and play into effects only after semi-convergence rather than from the very first iteration. If it works, the error norms of regularized solutions and the residual norms further decrease until they ultimately stabilize. The hybrid LSQR and CGME have been intensively studied in, e.g., [6,7,8,20,38,39,73,80,90] and [1,47,50]. Within the framework of such hybrid solvers, however, it is hard to find a near-optimal regularization parameter [13,90].

In contrast, if an iterative solver is theoretically proved and practically identified to have the full regularization, one simply stops it after semi-convergence, and no complicated hybrid variant and further iterations are needed. Obviously, we cannot emphasize too much the importance of proving the full or partial regularization of LSQR, CGLS, LSMR and CGME. By the definition of the full or partial regularization, we now modify the concern of Björck and Eldén as: Do LSQR, CGLS, LSMR and CGME have the full or partial regularization for severely, moderately and mildly ill-posed problems? How to identify their full or partial regularization in practice?

In this paper, we focus on LSQR and analyze its regularization for severely, moderately and mildly ill-posed problems. Due to the mathematical equivalence of CGLS and LSQR, the assertions on the full or partial regularization of LSQR apply to CGLS as well. We prove that LSQR has the full regularization for severely and moderately ill-posed problems once  $\rho > 1$  and  $\alpha > 1$  suitably, and it generally has only the partial regularization for mildly ill-posed problems. In Section 2, we describe the Lanczos bidiagonalization process and LSQR, and make an introductory analysis. In Section 3, we establish  $\sin \Theta$  theorems for the 2-norm distance between the underlying k-dimensional Krylov subspace and the k-dimensional dominant right singular subspace of A. We then derive some follow-up results that play a central role in analyzing the regularization of LSQR. In Section 4, for the first two kinds of problems we prove that a k-step Lanczos bidiagonalization always generates a near best rank k approximation to A, and the k Ritz values always approximate the first k large singular values in natural order, and no small Ritz value appears for  $k = 1, 2, \dots, k_0$ . This will show that LSQR has the full regularization. For mildly ill-posed problems, we prove that, for some  $k \le k_0$ , the k Ritz values generally do not approximate the first k large singular values in natural order and LSQR generally has only the partial regularization. In Section 5, we derive bounds for the entries of bidiagonal matrices generated by Lanczos bidiagonalization, showing how fast they decay and how to use them to identify if LSQR has the full regularization when the degree of ill-posedness of (1) is unknown in advance. In Section 6, we report numerical experiments to confirm our theory on LSQR. Finally, we summarize the paper with further remarks in Section 7.

Throughout the paper, we denote by  $\mathcal{K}_k(C, w) = span\{w, Cw, \dots, C^{k-1}w\}$  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  $|C| = (|c_{ij}|)$ ,  $|B| \le |C|$  means  $|b_{ij}| \le |c_{ij}|$  componentwise.

### 2 The LSQR algorithm

The LSQR algorithm is based on the Lanczos bidiagonalization process, Algorithm 1, that computes two orthonormal bases  $\{q_1, q_2, \dots, q_k\}$  and  $\{p_1, p_2, \dots, p_{k+1}\}$  of  $\mathcal{K}_k(A^TA, A^Tb)$ and  $\mathcal{K}_{k+1}(AA^T, b)$  for k = 1, 2, ..., n, respectively.

### Algorithm 1 k-step Lanczos bidiagonalization process

- 1. Take  $p_1 = b/||b|| \in \mathbb{R}^m$ , and define  $\beta_1 q_0 = 0$ .
- 2. For j = 1, 2, ..., 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)  $\beta_{i+1} = ||z||; p_{i+1} = z/\beta_{i+1}.$

Algorithm 1 can be written in the matrix form

$$AQ_k = P_{k+1}B_k, (12)$$

$$A^{T}P_{k+1} = Q_{k}B_{k}^{T} + \alpha_{k+1}q_{k+1}e_{k+1}^{T}.$$
(13)

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

$$B_{k} = \begin{pmatrix} \alpha_{1} \\ \beta_{2} & \alpha_{2} \\ \beta_{3} & \ddots \\ & \ddots & \alpha_{k} \\ & \beta_{k+1} \end{pmatrix} \in \mathbb{R}^{(k+1)\times k}. \tag{14}$$

It is known from (12) that

$$B_k = P_{k+1}^T A Q_k. (15)$$

We remind that the singular values 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.

At iteration k, LSQR solves the problem  $||Ax^{(k)} - b|| = \min_{x \in \mathcal{K}_k(A^T A, A^T b)} ||Ax - b||$ and computes the iterates  $x^{(k)} = Q_k y^{(k)}$  with

$$y^{(k)} = \arg\min_{y \in \mathbb{R}^k} \|B_k y - \|b\| e_1^{(k+1)} \| = \|b\| B_k^{\dagger} e_1^{(k+1)}, \tag{16}$$

where  $e_1^{(k+1)}$  is the first canonical basis vector of  $\mathbb{R}^{k+1}$ , and the residual norm  $||Ax^{(k)} - Ax^{(k)}||$ b decreases monotonically with respect to k. We have  $||Ax^{(k)} - b|| = ||B_ky^{(k)} - b||$  $||b||e_1^{(k+1)}||$  and  $||x^{(k)}|| = ||y^{(k)}||$ , both of which can be cheaply computed.

Note that  $||b||e_1^{(k+1)} = P_{k+1}^T b$ . We have

$$x^{(k)} = Q_k B_k^{\dagger} P_{k+1}^T b, \tag{17}$$

that is, the iterate  $x^{(k)}$  by LSQR is the minimum-norm least squares solution to the perturbed problem that replaces A in (1) by its rank k approximation  $P_{k+1}B_kQ_k^T$ . Recall that the best rank k approximation  $A_k$  to A satisfies  $||A-A_k|| = \sigma_{k+1}$ . Furthermore, analogous to (9), LSQR now solves

$$\min ||x|| \quad \text{subject to} \quad ||P_{k+1}B_kQ_k^Tx - b|| = \min, \ k = 1, 2, \dots, n$$
 (18)

for the regularized solutions  $x^{(k)}$  to (1). If  $P_{k+1}B_kQ_k^T$  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  $k=1,2,\ldots,k_0$ , these two facts relate LSQR and the TSVD method naturally and closely in two ways: (i)  $x_k^{tsvd}$  and  $x^{(k)}$  are the regularized solutions to the two perturbed problems of (1) that replace A by its two rank k approximations with the same quality, respectively; (ii)  $x_k^{tsvd}$  and  $x^{(k)}$  solve almost the same two regularization problems (9) and (18), respectively. As a consequence, the LSQR iterate  $x^{(k_0)}$  is as accurate as  $x_{k_0}^{tsvd}$ , and LSQR has the full regularization. Otherwise, as will be clear later, under the discrete Picard condition (7),  $x^{(k_0)}$  cannot be as accurate as  $x_{k_0}^{tsvd}$  if either  $P_{k+1}B_kQ_k^T$  is not a near best rank k approximation to A,  $k=1,2,\ldots,k_0$ , or  $B_k$  has at least one singular value smaller than  $\sigma_{k_0+1}$  for some  $k \leq k_0$ . Precisely, if either of them is violated for some  $k \leq k_0$  and  $\theta_k^{(k)} < \sigma_{k_0+1}$ ,  $x^{(k)}$  has been deteriorated by the noise e, and LSQR has only the partial regularization. We will give a precise definition of a near best rank k approximation to A soon

### 3 $\sin \Theta$ theorems for the distances between $\mathcal{K}_k(A^TA,A^Tb)$ and $span\{V_k\}$ as well as the others related

van der Sluis and van der Vorst [99] prove the following result, which has been used in Hansen [44] and the references therein to illustrate the regularizing effects of LSQR and CGLS. We will also investigate it further in our paper.

**Proposition 1** LSQR with the starting vector  $p_1 = b/\|b\|$  and CGLS applied to  $A^TAx = A^Tb$  with the starting vector  $x^{(0)} = 0$  generate the same iterates

$$x^{(k)} = \sum_{i=1}^{n} f_i^{(k)} \frac{u_i^T b}{\sigma_i} v_i, \ k = 1, 2, \dots, n,$$
 (19)

where

$$f_i^{(k)} = 1 - \prod_{j=1}^k \frac{(\theta_j^{(k)})^2 - \sigma_i^2}{(\theta_i^{(k)})^2}, \ i = 1, 2, \dots, n,$$
 (20)

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

(19) shows that  $x^{(k)}$  has a filtered SVD expansion of form (11). If all the Ritz values  $\theta_j^{(k)}$  approximate the first k singular values  $\sigma_j$  of A in natural order, the filters  $f_i^{(k)} \approx 1, i = 1, 2, ..., k$  and the other  $f_i^{(k)}$  monotonically approach zero for i = k + 1

 $1,\ldots,n$ . 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 the  $k_0$ -step LSQR has the full regularization. However, if a small Ritz value appears before some  $k \leq k_0$ , i.e.,  $\theta_{k-1}^{(k)} > \sigma_{k_0+1}$  and  $\sigma_{j^*} < \theta_k^{(k)} \leq \sigma_{k_0+1}$  with the smallest integer  $j^* > k_0+1$ , then  $f_i^{(k)} \in (0,1)$  tends to zero monotonically for  $i=j^*,j^*+1,\ldots,n$ ; on the other hand, we have

$$\prod_{j=1}^{k} \frac{(\theta_{j}^{(k)})^{2} - \sigma_{i}^{2}}{(\theta_{i}^{(k)})^{2}} = \frac{(\theta_{k}^{(k)})^{2} - \sigma_{i}^{2}}{(\theta_{k}^{(k)})^{2}} \prod_{j=1}^{k-1} \frac{(\theta_{j}^{(k)})^{2} - \sigma_{i}^{2}}{(\theta_{i}^{(k)})^{2}} \leq 0, \ i = k_{0} + 1, \dots, j^{*} - 1$$

since the first factor is non-positive and the second factor is positive. Then we get  $f_i^{(k)} \ge 1$ ,  $i = k_0 + 1, \dots, j^* - 1$ , indicating that  $x^{(k)}$  is already deteriorated and LSQR has only the partial regularization.

The standard k-step Lanczos bidiagonalization method computes the k Ritz values  $\theta_j^{(k)}$ , which are used to approximate some singular values of A. It is mathematically equivalent to the symmetric Lanczos method for the eigenvalue problem of  $A^TA$  starting with  $q_1 = A^Tb/\|A^Tb\|$ ; see [4,10,11,87,101] or [2,60,61] for several variations that are based on standard, harmonic, and refined projection [4,94,101] or a combination of them [59]. It is known that, for general singular value distribution and 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 converge slowly.

For (1),  $A^Tb$  contains more information on dominant right singular vectors than on the ones corresponding to small singular values. Therefore,  $\mathcal{K}_k(A^TA,A^Tb)$  hopefully contains richer information on the first k right singular vectors  $v_i$  than on the other n - k ones, at least for k small. Furthermore, note that A has many small singular values clustered at zero. Due to these two basic facts, all the Ritz values are expected to approximate the large singular values of A in natural order until some iteration k, at which a small Ritz value shows up. In this case, the iterates  $x^{(k)}$  by LSQR capture only the largest k dominant SVD components of A, and they are deteriorated by the noise e dramatically after that iteration. This is why LSQR and CGLS have general regularizing effects; see, e.g., [1,44,46,47,50] and the references therein. Unfortunately, these arguments cannot help us draw any definitive conclusion on the full or partial regularization of LSQR because there has been no quantitative result on the size of such k for any kind of ill-posed problem and the noise e. For a severely ill-posed example from seismic tomography, it is reported in [100] 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.

A complete understanding of the regularization of LSQR includes accurate solutions of the following problems: How accurately does  $\mathcal{K}_k(A^TA,A^Tb)$  approximate the k-dimensional dominant right singular subspace of A? How accurate is the rank k approximation  $P_{k+1}B_kQ_k^T$  to A? Can it be a near best rank k approximation to A? How does the noise level  $\|e\|$  affects the approximation accuracy of  $\mathcal{K}_k(A^TA,A^Tb)$  and  $P_{k+1}B_kQ_k^T$  for  $k \leq k_0$  and  $k > k_0$ , respectively? What sufficient conditions on p and p are needed to guarantee that  $p_{k+1}B_kQ_k^T$  is a near best rank k approximation to k?

When do the  $\theta_i^{(k)}$  approximate  $\sigma_i$ ,  $i=1,2,\ldots,k$  in natural order? When does at least a small Ritz value appear, i.e.,  $\theta_k^{(k)} < \sigma_{k_0+1}$  before some  $k \le k_0$ ? We will make a rigorous and detailed analysis on these problems, present our results, and draw definitive assertions on the regularization of LSQR for the three kinds of ill-posed problems.

In terms of the canonical angles  $\Theta(\mathcal{X}, \mathcal{Y})$  between two subspaces  $\mathcal{X}$  and  $\mathcal{Y}$  of equal dimension [95, p.43], we first present the following  $\sin \Theta$  theorem, showing how  $\mathcal{K}_k(A^TA, A^Tb)$  approximates the k-dimensional dominant right singular subspace  $span\{V_k\}$  of A for severely ill-posed problems.

**Theorem 1** Let the SVD of A be as (5). Assume that (1) is severely ill-posed with  $\sigma_j = \mathcal{O}(\rho^{-j})$  and  $\rho > 1$ , j = 1, 2, ..., n, and the discrete Picard condition (7) is satisfied. Let  $\mathcal{V}_k = span\{V_k\}$  be the k-dimensional dominant right singular subspace of A spanned by the columns of  $V_k = (v_1, v_2, ..., v_k)$  and  $\mathcal{V}_k^R = \mathcal{K}_k(A^T A, A^T b)$ . Then for k = 1, 2, ..., n-1 we have

$$\|\sin\Theta(\mathscr{V}_k,\mathscr{V}_k^R)\| = \frac{\|\Delta_k\|}{\sqrt{1+\|\Delta_k\|^2}},\tag{21}$$

$$\|\tan\Theta(\mathcal{V}_k,\mathcal{V}_k^R)\| = \|\Delta_k\| \tag{22}$$

with  $\Delta_k \in \mathbb{R}^{(n-k)\times k}$  to be defined by (30) and

$$\|\Delta_1\| \le \frac{\sigma_2}{\sigma_1} \frac{|u_2^T b|}{|u_1^T b|} (1 + \mathcal{O}(\rho^{-2})),$$
 (23)

$$\|\Delta_k\| \le \frac{\sigma_{k+1}}{\sigma_k} \frac{|u_{k+1}^T b|}{|u_k^T b|} \left(1 + \mathcal{O}(\rho^{-2})\right) |L_{k_1}^{(k)}(0)|, \ k = 2, 3, \dots, n-1, \tag{24}$$

where

$$|L_{k_1}^{(k)}(0)| = \max_{j=1,2,\dots,k} |L_j^{(k)}(0)|, \ |L_j^{(k)}(0)| = \prod_{i=1,i\neq j}^k \frac{\sigma_i^2}{|\sigma_j^2 - \sigma_i^2|}, \ j = 1, 2, \dots, k.$$
 (25)

In particular, we have

$$\|\Delta_1\| \le \frac{\sigma_2^{2+\beta}}{\sigma_1^{2+\beta}} \left(1 + \mathcal{O}(\rho^{-2})\right),\tag{26}$$

$$\|\Delta_k\| \le \frac{\sigma_{k+1}^{2+\beta}}{\sigma_k^{2+\beta}} \left(1 + \mathcal{O}(\rho^{-2})\right) |L_{k_1}^{(k)}(0)|, \ k = 2, 3, \dots, k_0, \tag{27}$$

$$\|\Delta_k\| \le \frac{\sigma_{k+1}}{\sigma_k} \left(1 + \mathcal{O}(\rho^{-2})\right) |L_{k_1}^{(k)}(0)|, \ k = k_0 + 1, \dots, n-1.$$
 (28)

*Proof.* Let  $U_n = (u_1, u_2, \dots, u_n)$  whose columns are the first n left singular vectors of A defined by (5). Then the Krylov subspace  $\mathcal{K}_k(\Sigma^2, \Sigma U_n^T b) = span\{DT_k\}$  with

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

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

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

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, ..., k, it is nonsingular. Therefore, from  $\mathscr{K}_k(A^TA, A^Tb) = span\{VDT_k\}$  we have

$$\mathscr{V}_{k}^{R} = \mathscr{K}_{k}(A^{T}A, A^{T}b) = span\left\{V\begin{pmatrix} D_{1}T_{k1} \\ D_{2}T_{k2} \end{pmatrix}\right\} = span\left\{V\begin{pmatrix} I \\ \Delta_{k} \end{pmatrix}\right\}, \quad (29)$$

where

$$\Delta_k = D_2 T_{k2} T_{k1}^{-1} D_1^{-1} \in \mathbb{R}^{(n-k) \times k}. \tag{30}$$

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

$$Z_k = V \begin{pmatrix} I \\ \Delta_k \end{pmatrix} = V_k + V_k^{\perp} \Delta_k. \tag{31}$$

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  $\mathcal{Y}_k^R$ . So we get an orthogonal direct sum decomposition of  $\hat{Z}_k$ :

$$\hat{Z}_k = (V_k + V_k^{\perp} \Delta_k) (I + \Delta_k^T \Delta_k)^{-\frac{1}{2}}.$$
(32)

By definition and (32), we obtain

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

which is (21). From it, we get (22) directly.

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  $\sigma_1^2, \sigma_2^2 \dots, \sigma_k^2$ . Consequently, the *j*-th column of  $T_{k2}T_{k1}^{-1}$  is

$$T_{k2}T_{k1}^{-1}e_i^{(k)} = (L_i^{(k)}(\sigma_{k+1}^2), \dots, L_i^{(k)}(\sigma_n^2))^T, \ j = 1, 2, \dots, k,$$
(33)

from which we obtain

$$T_{k2}T_{k1}^{-1} = \begin{pmatrix} L_1^{(k)}(\sigma_{k+1}^2) & L_2^{(k)}(\sigma_{k+1}^2) & \dots & L_k^{(k)}(\sigma_{k+1}^2) \\ L_1^{(k)}(\sigma_{k+2}^2) & L_2^{(k)}(\sigma_{k+2}^2) & \dots & L_k^{(k)}(\sigma_{k+2}^2) \\ \vdots & \vdots & & \vdots \\ L_1^{(k)}(\sigma_n^2) & L_2^{(k)}(\sigma_n^2) & \dots & L_k^{(k)}(\sigma_n^2) \end{pmatrix} \in \mathbb{R}^{(n-k)\times k}.$$
 (34)

Since  $|L_j^{(k)}(\lambda)|$  is monotonically decreasing for  $0 \le \lambda < \sigma_k^2$ , it is bounded by  $|L_j^{(k)}(0)|$ . With this property and the definition of  $L_{k_1}^{(k)}(0)$ , we get

$$\begin{split} |\Delta_{k}| &= |D_{2}T_{k2}T_{k1}^{-1}D_{1}^{-1}| \\ &\leq \begin{pmatrix} \frac{\sigma_{k+1}}{\sigma_{1}} \left| \frac{u_{k+1}^{T}b}{u_{1}^{T}b} \right| |L_{k_{1}}^{(k)}(0)| \frac{\sigma_{k+1}}{\sigma_{2}} \left| \frac{u_{k+1}^{T}b}{u_{2}^{T}b} \right| |L_{k_{1}}^{(k)}(0)| \dots \frac{\sigma_{k+1}}{\sigma_{k}} \left| \frac{u_{k+1}^{T}b}{u_{k}^{T}b} \right| |L_{k_{1}}^{(k)}(0)| \\ &\leq \frac{\sigma_{k+2}}{\sigma_{1}} \left| \frac{u_{k+2}^{T}b}{u_{1}^{T}b} \right| |L_{k_{1}}^{(k)}(0)| \frac{\sigma_{k+2}}{\sigma_{2}} \left| \frac{u_{k+2}^{T}b}{u_{2}^{T}b} \right| |L_{k_{1}}^{(k)}(0)| \dots \frac{\sigma_{k+2}}{\sigma_{k}} \left| \frac{u_{k+2}^{T}b}{u_{k}^{T}b} \right| |L_{k_{1}}^{(k)}(0)| \\ &\vdots &\vdots &\vdots \\ &\frac{\sigma_{n}}{\sigma_{1}} \left| \frac{u_{n}^{T}b}{u_{1}^{T}b} \right| |L_{k_{1}}^{(k)}(0)| \frac{\sigma_{n}}{\sigma_{2}} \left| \frac{u_{n}^{T}b}{u_{2}^{T}b} \right| |L_{k_{1}}^{(k)}(0)| \dots \frac{\sigma_{n}}{\sigma_{k}} \left| \frac{u_{n}^{T}b}{u_{k}^{T}b} \right| |L_{k_{1}}^{(k)}(0)| \\ &= |L_{k_{1}}^{(k)}(0)| |\tilde{\Delta}_{k}|, \end{split}$$

$$(35)$$

where

$$|\tilde{\Delta}_{k}| = \left| (\sigma_{k+1} u_{k+1}^{T} b, \sigma_{k+2} u_{k+2}^{T} b, \dots, \sigma_{n} u_{n}^{T} b)^{T} \left( \frac{1}{\sigma_{1} u_{1}^{T} b}, \frac{1}{\sigma_{2} u_{2}^{T} b}, \dots, \frac{1}{\sigma_{k} u_{k}^{T} b} \right) \right|$$
(36)

is a rank one matrix. Therefore, by  $||C|| \le |||C|||$  (cf. [93, p.53]), we get

$$\|\Delta_{k}\| \leq \||\Delta_{k}|\| \leq |L_{k_{1}}^{(k)}(0)| \||\tilde{\Delta}_{k}|\|$$

$$= |L_{k_{1}}^{(k)}(0)| \left(\sum_{j=k+1}^{n} \sigma_{j}^{2} |u_{j}^{T} b|^{2}\right)^{1/2} \left(\sum_{j=1}^{k} \frac{1}{\sigma_{j}^{2} |u_{j}^{T} b|^{2}}\right)^{1/2}.$$
(37)

By the discrete Picard condition (7), (8) and the description between them, for the white noise e, it is known from [44, p.70-1] and [47, p.41-2] that  $|u_j^Tb|\approx |u_j^T\hat{b}|=\sigma_j^{1+\beta}$  decrease as j increases up to  $k_0$  and then become stabilized as  $|u_j^Tb|\approx |u_j^Te|\approx \eta\approx \frac{\|e\|}{\sqrt{m}}$ , a small constant for  $j>k_0$ . In order to simplify the derivation and present our results compactly, in terms of these assumptions and properties, in later proofs we will use the following strict equalities and inequalities:

$$|u_j^T b| = |u_j^T \hat{b}| = \sigma_j^{1+\beta}, \ j = 1, 2, \dots, k_0,$$
 (38)

$$|u_j^T b| = |u_j^T e| = \eta, \ j = k_0 + 1, \dots, n,$$
 (39)

$$|u_{j+1}^T b| \le |u_j^T b|, \ j = 1, 2, \dots, n-1.$$
 (40)

From (40) and  $\sigma_j = \mathcal{O}(\rho^{-j}), j = 1, 2, \dots, n$ , for  $k = 1, 2, \dots, n-1$  we obtain

$$\left(\sum_{j=k+1}^{n} \sigma_{j}^{2} | u_{j}^{T} b|^{2}\right)^{1/2} = \sigma_{k+1} | u_{k+1}^{T} b| \left(\sum_{j=k+1}^{n} \frac{\sigma_{j}^{2} | u_{j}^{T} b|^{2}}{\sigma_{k+1}^{2} | u_{k+1}^{T} b|^{2}}\right)^{1/2} \\
\leq \sigma_{k+1} | u_{k+1}^{T} b| \left(\sum_{j=k+1}^{n} \frac{\sigma_{j}^{2}}{\sigma_{k+1}^{2}}\right)^{1/2} \\
= \sigma_{k+1} | u_{k+1}^{T} b| \left(1 + \sum_{j=k+2}^{n} \mathscr{O}(\rho^{2(k-j)+2})\right)^{1/2} \\
= \sigma_{k+1} | u_{k+1}^{T} b| \left(1 + \mathscr{O}\left(\sum_{j=k+2}^{n} \rho^{2(k-j)+2}\right)\right)^{1/2} \\
= \sigma_{k+1} | u_{k+1}^{T} b| \left(1 + \mathscr{O}\left(\frac{\rho^{-2}}{1 - \rho^{-2}}\left(1 - \rho^{-2(n-k-1)}\right)\right)\right)^{1/2} \\
= \sigma_{k+1} | u_{k+1}^{T} b| \left(1 + \mathscr{O}(\rho^{-2})\right)^{1/2} \\
= \sigma_{k+1} | u_{k+1}^{T} b| \left(1 + \mathscr{O}(\rho^{-2})\right) \tag{41}$$

with  $1 + \mathcal{O}(\rho^{-2}) = 1$  for k = n - 1. For k = 2, 3, ..., n - 1, from (40) we get

$$\begin{split} \left(\sum_{j=1}^{k} \frac{1}{\sigma_{j}^{2} |u_{j}^{T} b|^{2}}\right)^{1/2} &= \frac{1}{\sigma_{k} |u_{k}^{T} b|} \left(\sum_{j=1}^{k} \frac{\sigma_{k}^{2} |u_{k}^{T} b|^{2}}{\sigma_{j}^{2} |u_{j}^{T} b|^{2}}\right)^{1/2} \leq \frac{1}{\sigma_{k} |u_{k}^{T} b|} \left(\sum_{j=1}^{k} \frac{\sigma_{k}^{2}}{\sigma_{j}^{2}}\right)^{1/2} \\ &= \frac{1}{\sigma_{k} |u_{k}^{T} b|} \left(1 + \mathcal{O}\left(\sum_{j=1}^{k-1} \rho^{2(j-k)}\right)\right)^{1/2} \\ &= \frac{1}{\sigma_{k} |u_{k}^{T} b|} \left(1 + \mathcal{O}(\rho^{-2})\right). \end{split}$$

From the above and (37), we finally obtain (24) by noting

$$\|\Delta_k\| \leq \frac{\sigma_{k+1}}{\sigma_k} \frac{|u_{k+1}^T b|}{|u_k^T b|} \left(1 + \mathscr{O}(\rho^{-2})\right) |L_{k_1}^{(k)}(0)|, \ k = 2, 3, \dots, n-1.$$

Note that the Lagrange polynomials  $L_j^{(k)}(\lambda)$  require  $k \geq 2$ . So, we need to treat the case k=1 independently. Observe from (30) and (40) that

$$T_{k2} = (1, 1, \dots, 1)^T, D_2 T_{k2} = (\sigma_2 u_2^T b, \sigma_3 u_3^T b, \dots, \sigma_n u_n^T b)^T, T_{k1}^{-1} = 1, D_1^{-1} = \frac{1}{\sigma_1 u_1^T b}.$$

Therefore, we have

$$\Delta_1 = (\sigma_2 u_2^T b, \sigma_3 u_3^T b, \dots, \sigma_n u_n^T b)^T \frac{1}{\sigma_1 u_1^T b},$$
(42)

from which and (41) for k = 1 it is direct to get (23).

In terms of the discrete Picard condition (7), (8), (38) and (39), we have

$$\frac{|u_{k+1}^T b|}{|u_k^T b|} = \frac{|u_{k+1}^T \hat{b}|}{|u_k^T \hat{b}|} = \frac{\sigma_{k+1}^{1+\beta}}{\sigma_k^{1+\beta}}, \ k \le k_0, \tag{43}$$

$$\frac{|u_{k+1}^T b|}{|u_k^T b|} = \frac{|u_{k+1}^T e|}{|u_k^T e|} = 1, \ k > k_0.$$
(44)

Applying them to (23) and (24) establishes (26), (27) and (28), respectively.  $\Box$  We next estimate the factor  $|L_{k_1}^{(k)}(0)|$  and all  $|L_j^{(k)}(0)|$ ,  $j=1,2,\ldots,k$  accurately.

**Theorem 2** For the severely ill-posed problem, we have

$$|L_k^{(k)}(0)| = 1 + \mathcal{O}(\rho^{-2}),$$
 (45)

$$|L_j^{(k)}(0)| = \frac{1 + \mathcal{O}(\rho^{-2})}{\prod\limits_{i=j+1}^k \left(\frac{\sigma_j}{\sigma_i}\right)^2} = \frac{1 + \mathcal{O}(\rho^{-2})}{\mathcal{O}(\rho^{(k-j)(k-j+1)})}, \ j = 1, 2, \dots, k-1,$$
(46)

$$|L_{k_1}^{(k)}(0)| = \max_{j=1,2,\dots,k} |L_j^{(k)}(0)| = 1 + \mathcal{O}(\rho^{-2}). \tag{47}$$

*Proof.* Exploiting the Taylor series expansion and  $\sigma_i = \mathcal{O}(\rho^{-i})$  for i = 1, 2, ..., n, by definition, for j = 1, 2, ..., k - 1 we have

$$|L_{j}^{(k)}(0)| = \prod_{i=1, i \neq j}^{k} \left| \frac{\sigma_{i}^{2}}{\sigma_{i}^{2} - \sigma_{j}^{2}} \right| = \prod_{i=1}^{j-1} \frac{\sigma_{i}^{2}}{\sigma_{i}^{2} - \sigma_{j}^{2}} \cdot \prod_{i=j+1}^{k} \frac{\sigma_{i}^{2}}{\sigma_{j}^{2} - \sigma_{i}^{2}}$$

$$= \prod_{i=1}^{j-1} \frac{1}{1 - \mathcal{O}(\rho^{-2(j-i)})} \prod_{i=j+1}^{k} \frac{1}{1 - \mathcal{O}(\rho^{-2(i-j)})} \frac{1}{\prod_{i=j+1}^{k} \mathcal{O}(\rho^{2(i-j)})}$$

$$= \frac{\left(1 + \sum_{i=1}^{j} \mathcal{O}(\rho^{-2i})\right) \left(1 + \sum_{i=1}^{k-j+1} \mathcal{O}(\rho^{-2i})\right)}{\prod_{i=j+1}^{k} \mathcal{O}(\rho^{2(i-j)})}$$
(48)

by absorbing those higher order terms into  $\mathcal{O}(\cdot)$  in the numerator. For j = k, we get

$$\begin{split} |L_k^{(k)}(0)| &= \prod_{i=1}^{k-1} \left| \frac{\sigma_i^2}{\sigma_i^2 - \sigma_k^2} \right| = \prod_{i=1}^{k-1} \frac{1}{1 - \mathcal{O}(\rho^{-2(k-i)})} = \prod_{i=1}^{k-1} \frac{1}{1 - \mathcal{O}(\rho^{-2i})} \\ &= 1 + \sum_{i=1}^k \mathcal{O}(\rho^{-2i}) = 1 + \mathcal{O}\left(\sum_{i=1}^k \rho^{-2i}\right) \\ &= 1 + \mathcal{O}\left(\frac{\rho^{-2}}{1 - \rho^{-2}}(1 - \rho^{-2k})\right) = 1 + \mathcal{O}(\rho^{-2}), \end{split}$$

which is (45).

Note that for the numerator of (48) we have

$$1 + \sum_{i=1}^{j} \mathscr{O}(\rho^{-2i}) = 1 + \mathscr{O}\left(\sum_{i=1}^{j} \rho^{-2i}\right) = 1 + \mathscr{O}\left(\frac{\rho^{-2}}{1 - \rho^{-2}}(1 - \rho^{-2j})\right),$$

and

$$1 + \sum_{i=1}^{k-j+1} \mathscr{O}(\rho^{-2i}) = 1 + \mathscr{O}\left(\sum_{i=1}^{k-j+1} \rho^{-2i}\right) = 1 + \mathscr{O}\left(\frac{\rho^{-2}}{1-\rho^{-2}}(1-\rho^{-2(k-j+1)})\right),$$

whose product for any k is

$$1 + \mathcal{O}\left(\frac{2\rho^{-2}}{1 - \rho^{-2}}\right) + \mathcal{O}\left(\left(\frac{\rho^{-2}}{1 - \rho^{-2}}\right)^{2}\right) = 1 + \mathcal{O}\left(\frac{2\rho^{-2}}{1 - \rho^{-2}}\right) = 1 + \mathcal{O}(\rho^{-2}).$$

On the other hand, note that the denominator of (48) is defined by

$$\prod_{i=j+1}^k \left(\frac{\sigma_j}{\sigma_i}\right)^2 = \prod_{i=j+1}^k \mathscr{O}(\rho^{2(i-j)}) = \mathscr{O}((\rho \cdot \rho^2 \cdots \rho^{k-j})^2) = \mathscr{O}(\rho^{(k-j)(k-j+1)}),$$

which, together with the above estimate for the numerator of (48), proves (46). Notice that the above quantity is always *bigger than one* for j = 1, 2, ..., k - 1. Therefore, for any k, combining (45) and (46) gives (47).

Remark 1 From (47), the results in Theorem 1 are simplified as

$$\|\Delta_k\| \le \frac{\sigma_{k+1}^{2+\beta}}{\sigma_k^{2+\beta}} \left(1 + \mathcal{O}(\rho^{-2})\right), \ k = 1, 2, \dots, k_0,$$
 (49)

$$\|\Delta_k\| \le \frac{\sigma_{k+1}}{\sigma_k} \left( 1 + \mathcal{O}(\rho^{-2}) \right), \ k = k_0 + 1, \dots, n-1.$$
 (50)

Remark 2 It is seen from the proof that  $k_1$  must be close to k or equals k. (46) illustrates that  $|L_j^{(k)}(0)|$  increases fast, up to  $1+\mathcal{O}(\rho^{-2})$ , with j increasing, and the smaller j, the smaller  $|L_j^{(k)}(0)|$ . (49) and (50) indicate that  $\mathcal{V}_k^R$  captures  $\mathcal{V}_k$  better for  $k \leq k_0$  than for  $k > k_0$ . That is, after iteration  $k_0$ , the noise e starts to impair the ability of  $\mathcal{V}_k^R$  to capture  $\mathcal{V}_k$ .

Next we estimate  $\|\sin\Theta(\mathscr{V}_k,\mathscr{V}_k^R)\|$  for moderately and mildly ill-posed problems.

**Theorem 3** Assume that (1) is moderately or mildly ill-posed with  $\sigma_j = \zeta j^{-\alpha}$ , j = 1, 2, ..., n, where  $\alpha > \frac{1}{2}$  and  $\zeta > 0$  is some constant. Then (21) and (22) hold with

$$\|\Delta_1\| \le \frac{\sigma_2^{1+\beta}}{\sigma_1^{1+\beta}} \sqrt{\frac{1}{2\alpha - 1}},$$
 (51)

$$\|\Delta_k\| \le \frac{\sigma_{k+1}^{1+\beta}}{\sigma_k^{1+\beta}} \sqrt{\frac{k^2}{4\alpha^2 - 1} + \frac{k}{2\alpha - 1}} |L_{k_1}^{(k)}(0)|, \ k = 2, 3, \dots, k_0,$$
 (52)

$$\|\Delta_k\| \le \sqrt{\frac{k^2}{4\alpha^2 - 1} + \frac{k}{2\alpha - 1}} |L_{k_1}^{(k)}(0)|, \ k = k_0 + 1, \dots, n - 1.$$
 (53)

*Proof.* Following the proof of Theorem 1, we know that  $|\Delta_k| \leq |L_{k_1}^{(k)}(0)||\tilde{\Delta}_k|$  still holds with  $\tilde{\Delta}_k$  defined by (36). So we only need to bound the right-hand side of (37). For  $k = 1, 2, \ldots, n-1$ , from (40) we get

$$\left(\sum_{j=k+1}^{n} \sigma_{j}^{2} | u_{j}^{T} b|^{2}\right)^{1/2} = \sigma_{k+1} | u_{k+1}^{T} b| \left(\sum_{j=k+1}^{n} \frac{\sigma_{j}^{2} | u_{j}^{T} b|^{2}}{\sigma_{k+1}^{2} | u_{k+1}^{T} b|^{2}}\right)^{1/2}$$

$$\leq \sigma_{k+1} | u_{k+1}^{T} b| \left(\sum_{j=k+1}^{n} \frac{\sigma_{j}^{2}}{\sigma_{k+1}^{2}}\right)^{1/2}$$

$$= \sigma_{k+1} | u_{k+1}^{T} b| \left(\sum_{j=k+1}^{n} \left(\frac{j}{k+1}\right)^{-2\alpha}\right)^{1/2}$$

$$= \sigma_{k+1} | u_{k+1}^{T} b| \left((k+1)^{2\alpha} \sum_{j=k+1}^{n} \frac{1}{j^{2\alpha}}\right)^{1/2}$$

$$< \sigma_{k+1} | u_{k+1}^{T} b| (k+1)^{\alpha} \left(\int_{k}^{\infty} \frac{1}{x^{2\alpha}} dx\right)^{1/2}$$

$$= \sigma_{k+1} | u_{k+1}^{T} b| \left(\frac{k+1}{k}\right)^{\alpha} \sqrt{\frac{k}{2\alpha-1}}$$

$$= \sigma_{k+1} | u_{k+1}^{T} b| \frac{\sigma_{k}}{\sigma_{k+1}} \sqrt{\frac{k}{2\alpha-1}}.$$

$$= \sigma_{k} | u_{k+1}^{T} b| \sqrt{\frac{k}{2\alpha-1}}.$$
(54)

Since the function  $x^{2\alpha}$  with any  $\alpha > \frac{1}{2}$  is convex over the interval [0,1], for  $k = 2,3,\ldots,n-1$ , from (40) we obtain

$$\left(\sum_{j=1}^{k} \frac{1}{\sigma_{j}^{2} |u_{j}^{T} b|^{2}}\right)^{1/2} = \frac{1}{\sigma_{k} |u_{k}^{T} b|} \left(\sum_{j=1}^{k} \frac{\sigma_{k}^{2} |u_{k}^{T} b|^{2}}{\sigma_{j}^{2} |u_{j}^{T} b|^{2}}\right)^{1/2} \leq \frac{1}{\sigma_{k} |u_{k}^{T} b|} \left(\sum_{j=1}^{k} \frac{\sigma_{k}^{2}}{\sigma_{j}^{2}}\right)^{2}$$

$$= \frac{1}{\sigma_{k} |u_{k}^{T} b|} \left(\sum_{j=1}^{k} \left(\frac{j}{k}\right)^{2\alpha}\right)^{1/2}$$

$$= \frac{1}{\sigma_{k} |u_{k}^{T} b|} \left(k \sum_{j=1}^{k} \frac{1}{k} \left(\frac{j-1}{k}\right)^{2\alpha} + 1\right)^{1/2}$$

$$< \frac{1}{\sigma_{k} |u_{k}^{T} b|} \left(k \int_{0}^{1} x^{2\alpha} dx + 1\right)^{1/2}$$

$$= \frac{1}{\sigma_{k} |u_{k}^{T} b|} \sqrt{\frac{k}{2\alpha + 1} + 1}.$$
(55)

Substituting the above and (54) into (37) and exploiting (43) and (44), we obtain (52) and (53). For k = 1, it follows from (42) and (43) that (51) holds.

Remark 3 For the sake of precise presentation, we have used the simplified singular value model  $\sigma_j = \zeta j^{-\alpha}$  to replace the general form  $\sigma_j = \mathcal{O}(j^{-\alpha})$ , where the constant in each  $\mathcal{O}(\cdot)$  is implicit. This model, though simple, reflects the essence of moderately and mildly ill-posed problems and avoids some non-transparent formulations.

Unlike the severely ill-posed problem case, for moderately and mildly ill-posed problems it appears impossible to estimate  $|L_{k_1}^{(k)}(0)|$  both elegantly and accurately. We present the following results on  $|L_j^{(k)}(0)|$ ,  $j=1,2,\ldots,k$  and  $|L_{k_1}^{(k)}(0)|$ .

**Proposition 2** For the moderately and mildly ill-posed problems with  $\sigma_i = \zeta i^{-\alpha}$ , i = 1, 2, ..., n and  $\alpha > \frac{1}{2}$ , we have

$$|L_k^{(k)}(0)| \approx 1 + \frac{k}{2\alpha + 1},$$
 (57)

$$|L_{j}^{(k)}(0)| \approx \left(1 + \frac{j}{2\alpha + 1}\right) \left(1 + \frac{j - j^{2\alpha}k^{-2\alpha + 1}}{2\alpha - 1}\right) \prod_{i=j+1}^{k} \left(\frac{j}{i}\right)^{2\alpha}, j = 1, 2, \dots, k - 1.$$
(58)

For  $\alpha > 1$ , we have

$$|L_j^{(k)}(0)| \approx \left(1 + \frac{j}{2\alpha + 1}\right) \prod_{i=j+1}^k \left(\frac{j}{i}\right)^{2\alpha}, j = 1, 2, \dots, k-1,$$
 (59)

$$\frac{k}{2\alpha+1} < |L_{k_1}^{(k)}(0)| \approx 1 + \frac{k}{2\alpha+1} \tag{60}$$

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

$$\frac{k}{2\alpha+1} < |L_{k_1}^{(k)}(0)|. \tag{61}$$

*Proof.* Exploiting the first order Taylor expansion, we obtain estimate

$$\begin{split} |L_k^{(k)}(0)| &= \prod_{i=1}^{k-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_k^2} = \prod_{i=1}^{k-1} \frac{1}{1 - (\frac{i}{k})^{2\alpha}} \\ &\approx 1 + \sum_{i=1}^{k-1} \left(\frac{i}{k}\right)^{2\alpha} = 1 + k \sum_{i=1}^k \frac{1}{k} \left(\frac{i-1}{k}\right)^{2\alpha} \\ &\approx 1 + k \int_0^1 x^{2\alpha} dx = 1 + \frac{k}{2\alpha + 1}, \end{split}$$

which proves (57).

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

$$\begin{split} |L_{j}^{(k)}(0)| &= \prod_{i=1, i \neq j}^{k} \left| \frac{\sigma_{i}^{2}}{\sigma_{i}^{2} - \sigma_{j}^{2}} \right| = \prod_{i=1}^{j-1} \frac{\sigma_{i}^{2}}{\sigma_{i}^{2} - \sigma_{j}^{2}} \cdot \prod_{i=j+1}^{k} \frac{\sigma_{i}^{2}}{\sigma_{j}^{2} - \sigma_{i}^{2}} \\ &= \prod_{i=1}^{j-1} \frac{1}{1 - \left(\frac{i}{j}\right)^{2\alpha}} \prod_{i=j+1}^{k} \frac{1}{1 - \left(\frac{j}{i}\right)^{2\alpha}} \frac{1}{\prod_{i=j+1}^{k} \left(\frac{i}{j}\right)^{2\alpha}} \\ &\approx \left(1 + \sum_{i=1}^{j-1} \left(\frac{i}{j}\right)^{2\alpha}\right) \left(1 + \sum_{i=j+1}^{k} \left(\frac{j}{i}\right)^{2\alpha}\right) \prod_{i=j+1}^{k} \left(\frac{j}{i}\right)^{2\alpha} \\ &\leq \left(1 + \int_{0}^{1} x^{2\alpha} dx\right) \left(1 + j^{2\alpha} \int_{j}^{k} \frac{1}{x^{2\alpha}} dx\right) \prod_{i=j+1}^{k} \left(\frac{j}{i}\right)^{2\alpha} \\ &= \left(1 + \frac{j}{2\alpha + 1}\right) \left(1 + \frac{j - j^{2\alpha}k^{-2\alpha + 1}}{2\alpha - 1}\right) \prod_{i=j+1}^{k} \left(\frac{j}{i}\right)^{2\alpha}. \end{split}$$

Note that  $\prod_{i=j+1}^k \left(\frac{j}{i}\right)^{2\alpha}$  are always smaller than one for  $j=1,2,\ldots,k-1$ , and the smaller j is, the smaller this factor is. Furthermore, exploiting

$$\left(\frac{j}{k}\right)^{k-j} < \prod_{i=j+1}^{k} \frac{j}{i} < \left(\frac{j}{j+1}\right)^{k-j}$$

and by some elementary manipulation, for  $\alpha > 1$  we can justify the estimates

$$\frac{j - j^{2\alpha}k^{-2\alpha+1}}{2\alpha - 1} \prod_{i=j+1}^{k} \left(\frac{j}{i}\right)^{2\alpha} \approx 0, \ j = 1, 2, \dots, k-1.$$

As a result, for  $\alpha > 1$  we have

$$|L_j^{(k)}(0)|pprox \left(1+rac{j}{2lpha+1}
ight)\prod_{i=j+1}^k \left(rac{j}{i}
ight)^{2lpha},\, j=1,2,\ldots,k-1,$$

which establishes (59). A combination of it and (57) gives the right-hand part of (60). On the other hand, once k is such that  $\frac{2\alpha+1}{k} \le 1$ , we always have

$$|L_{k_1}^{(k)}(0)| \ge |L_k^{(k)}(0)| = \prod_{i=1}^{k-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_k^2} = \prod_{i=1}^{k-1} \frac{1}{1 - (\frac{i}{k})^{2\alpha}}$$

$$> 1 + \sum_{i=1}^{k-1} \left(\frac{i}{k}\right)^{2\alpha} > 1 + k \int_0^{\frac{k-1}{k}} x^{2\alpha} dx$$

$$= 1 + \frac{k\left(\frac{k-1}{k}\right)^{2\alpha+1}}{2\alpha+1} \approx 1 + \frac{k}{2\alpha+1} \left(1 - \frac{2\alpha+1}{k}\right) = \frac{k}{2\alpha+1}, \tag{62}$$

which yields the lower bound of (60) and (61).

Remark 4 The inaccuracy source of (57) and (58) consists in using  $\Sigma$  to replace  $\Pi$  approximately in the proof. They are considerable underestimates for  $\frac{1}{2} < \alpha \le 1$  but are accurate, provided that  $\alpha > 1$  suitably; the bigger  $\alpha$  is, the more accurate the estimates (57) and (58) are. The derivation of (62) indicates that  $|L_{k_1}^{(k)}(0)|$  can be bigger than  $\frac{k}{2\alpha+1}$  substantially for  $\frac{1}{2} < \alpha \le 1$ , particularly when  $\alpha$  is close to  $\frac{1}{2}$ ; in this case, we cannot bound  $|L_{k_1}^{(k)}(0)|$  from above since (58) is a considerable underestimate and the denominator  $2\alpha-1$  in (58) can be very small.

Remark 5 It is easily seen from (21) that  $\|\sin\Theta(\mathcal{V}_k,\mathcal{V}_k^R)\|$  increases monotonically with respect to  $\|\Delta_k\|$ . For  $\|\Delta_k\|$  reasonably small and  $\|\Delta_k\|$  large we have

$$\|\sin\Theta(\mathscr{V}_k,\mathscr{V}_k^R)\| \approx \|\Delta_k\|$$
 and  $\|\sin\Theta(\mathscr{V}_k,\mathscr{V}_k^R)\| \approx 1$ ,

respectively. From (7) and (8), we obtain  $k_0 = \lfloor \eta^{-\frac{1}{\alpha(1+\beta)}} \rfloor - 1$ , where  $\lfloor \cdot \rfloor$  is the Gaussian function. As a result, for  $\alpha > 1$ ,  $k_0$  is typically small and at most modest for a practical noise e with  $\|e\| \approx \sqrt{m\eta}$  since  $\frac{\|e\|}{\|\hat{b}\|}$  typically ranges from  $10^{-4}$  to  $10^{-2}$ . This means that for a moderately ill-posed problem  $\|\Delta_k\|$  is at most modest and cannot be large, so that  $\|\sin\Theta(\mathcal{V}_k,\mathcal{V}_k^R)\| < 1$  fairly.

Remark 6 For severely ill-posed problems, since all the  $\frac{\sigma_{k+1}}{\sigma_k} \sim \rho^{-1}$ , (49) and (50) indicate that  $\|\sin\Theta(\mathcal{V}_k,\mathcal{V}_k^R)\|$  is essentially unchanged for  $k=1,2,\ldots,k_0$  and  $k=k_0+1,\ldots,n-1$ , respectively, meaning that  $\mathcal{V}_k^R$  captures  $\mathcal{V}_k$  with almost the same accuracy for  $k\leq k_0$  and  $k>k_0$ , respectively. However, the situation is different for moderately ill-posed problems. For them,  $\frac{\sigma_{k+1}}{\sigma_k} = \left(\frac{k}{k+1}\right)^\alpha$  increases slowly as k increases, and  $\sqrt{\frac{k^2}{4\alpha^2-1} + \frac{k}{2\alpha-1}}|L_{k_1}^{(k)}(0)|$  increases as k grows. Therefore, (52) and (53) illustrate that  $\|\sin\Theta(\mathcal{V}_k,\mathcal{V}_k^R)\|$  increases slowly with  $k\leq k_0$  and  $k>k_0$ , respectively. This means that  $\mathcal{V}_k^R$  may not capture  $\mathcal{V}_k$  so well as it does for severely ill-posed problems as k increases. In particular, starting with some  $k>k_0$ ,  $\|\sin\Theta(\mathcal{V}_k,\mathcal{V}_k^R)\|$  starts to approach one, which indicates that, for k big,  $\mathcal{V}_k^R$  will contain substantial information on the right singular vectors corresponding to the n-k small singular values of A.

Remark 7 For mildly ill-posed problems with  $\frac{1}{2} < \alpha \le 1$ , there are some distinctive features. Note from (7) and (8) that  $k_0$  is now considerably bigger than that for a severely or moderately ill-posed problem with the same noise level  $\|e\|$  and  $\beta$ . As a result, firstly, for  $\alpha \le 1$  and the same k, the factor  $\frac{\sigma_{k+1}}{\sigma_k} = \left(\frac{k}{k+1}\right)^{\alpha}$  is bigger than that for the moderately ill-posed problem; secondly,  $\sqrt{\frac{k^2}{4\alpha^2-1} + \frac{k}{2\alpha-1}} \sim k$  if  $\alpha \approx 1$  and is much bigger than k and can be arbitrarily large if  $\alpha \approx \frac{1}{2}$ ; thirdly, (62) and the comment on it indicate that  $|L_{k_1}^{(k)}(0)|$  is bigger than one considerably for  $\frac{1}{2} < \alpha \le 1$  as k increases up to  $k_0$ . The bound (52) thus becomes increasingly large as k increases up to  $k_0$  for mildly ill-posed problems, causing that  $\|\Delta_k\|$  is large and  $\|\sin\Theta(\mathcal{V}_k,\mathcal{V}_k^R)\| \approx 1$  starting with some  $k \le k_0$ . Consequently,  $\mathcal{V}_{k_0}^R$  cannot effectively capture  $\mathcal{V}_{k_0}$  and contains substantial information on the right singular vectors corresponding to the  $n-k_0$  small singular values.

Before proceeding, we tentatively investigate how  $\|\sin\Theta(\mathscr{V}_k,\mathscr{V}_k^R)\|$  affects the smallest Ritz value  $\theta_k^{(k)}$ . This problem is of central importance for understanding the regularizing effects of LSQR. We aim to lead the reader to a first manifestation that (i) we may have  $\theta_k^{(k)} > \sigma_{k+1}$ , that is, no small Ritz value may appear when  $\|\sin\Theta(\mathscr{V}_k,\mathscr{V}_k^R)\| < 1$  suitably, and (ii) we must have  $\theta_k^{(k)} \leq \sigma_{k+1}$ , that is,  $\theta_k^{(k)}$  cannot approximate  $\sigma_k$  in natural order, meaning that  $\theta_k^{(k)} \leq \sigma_{k_0+1}$  no later than iteration  $k_0$ , once  $\|\sin\Theta(\mathscr{V}_k,\mathscr{V}_k^R)\|$  is sufficiently close to one.

**Theorem 4** Let  $\|\sin\Theta(\mathcal{V}_k,\mathcal{V}_k^R)\|^2 = 1 - \varepsilon_k^2$  with  $0 < \varepsilon_k < 1$ ,  $k = 1,2,\ldots,n-1$ , and let the unit-length  $\tilde{q}_k \in \mathcal{V}_k^R$  be a vector that has the smallest acute angle with span $\{V_k^\perp\}$ , i.e., the closest to span $\{V_k^\perp\}$ , where  $V_k^\perp$  is the matrix consisting of the last n-k columns of V defined by (5). Then it holds that

$$\varepsilon_k^2 \sigma_k^2 + (1 - \varepsilon_k^2) \sigma_n^2 < \tilde{q}_k^T A^T A \tilde{q}_k < \varepsilon_k^2 \sigma_{k+1}^2 + (1 - \varepsilon_k^2) \sigma_1^2. \tag{63}$$

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

$$\sqrt{\tilde{q}_k^T A^T A \tilde{q}_k} > \sigma_{k+1}; \tag{64}$$

if  $\varepsilon_k^2 \leq \frac{\delta}{(\frac{\sigma_1}{\sigma_{k+1}})^2-1}$  for a given arbitrarily small  $\delta>0$ , then

$$\theta_{\nu}^{(k)} < (1+\delta)^{1/2} \sigma_{k+1}.$$
 (65)

*Proof.* Since the columns of  $Q_k$  generated by Lanczos bidiagonalization form an orthonormal basis of  $\mathcal{V}_k^R$ , by definition and the assumption on  $\tilde{q}_k$  we have

$$\|\sin\Theta(\mathscr{V}_{k},\mathscr{V}_{k}^{R})\| = \|(V_{k}^{\perp})^{T}Q_{k}\| = \|V_{k}^{\perp}(V_{k}^{\perp})^{T}Q_{k}\|$$

$$= \max_{\|c\|=1} \|V_{k}^{\perp}(V_{k}^{\perp})^{T}Q_{k}c\| = \|V_{k}^{\perp}(V_{k}^{\perp})^{T}Q_{k}c_{k}\|$$

$$= \|V_{k}^{\perp}(V_{k}^{\perp})^{T}\tilde{q}_{k}\| = \|(V_{k}^{\perp})^{T}\tilde{q}_{k}\| = \sqrt{1 - \varepsilon_{k}^{2}}$$
(66)

with  $\tilde{q}_k = Q_k c_k \in \mathscr{V}_k^R$  and  $||c_k|| = 1$ . Since  $\mathscr{V}_k$  is the orthogonal complement of  $span\{V_k^{\perp}\}$ , by definition we know that  $\tilde{q}_k \in \mathscr{V}_k^R$  has the largest acute angle with  $\mathscr{V}_k$ , that is, it is the vector in  $\mathscr{V}_k^R$  that contains the least information on  $\mathscr{V}_k$ .

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

$$\tilde{q}_k = V_{\iota}^{\perp} (V_{\iota}^{\perp})^T \tilde{q}_k + V_{\iota} V_{\iota}^T \tilde{q}_k. \tag{67}$$

Then from  $\|\tilde{q}_k\| = 1$  and (66) we obtain

$$\|V_k^T \tilde{q}_k\| = \|V_k V_k^T \tilde{q}_k\| = \sqrt{1 - \|V_k^{\perp} (V_k^{\perp})^T \tilde{q}_k\|^2} = \sqrt{1 - (1 - \varepsilon_k^2)} = \varepsilon_k.$$
 (68)

From (67), we next bound the Rayleigh quotient of  $\tilde{q}_k$  with respect to  $A^TA$  from below. By the SVD (5) of A and  $V = (V_k, V_k^{\perp})$ , we partition

$$\Sigma = \left(egin{array}{c} \Sigma_k \ \Sigma_k^\perp \end{array}
ight),$$

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

$$\begin{split} \tilde{q}_k^T A^T A \tilde{q}_k &= \left( V_k^{\perp} (V_k^{\perp})^T \tilde{q}_k + V_k V_k^T \tilde{q}_k \right)^T A^T A \left( V_k^{\perp} (V_k^{\perp})^T \tilde{q}_k + V_k V_k^T \tilde{q}_k \right) \\ &= \left( \tilde{q}_k^T V_k^{\perp} (V_k^{\perp})^T + \tilde{q}_k^T V_k V_k^T \right) \left( V_k^{\perp} (\Sigma_k^{\perp})^2 (V_k^{\perp})^T \tilde{q}_k + V_k \Sigma_k^2 V_k^T \tilde{q}_k \right) \\ &= \tilde{q}_k^T V_k^{\perp} (\Sigma_k^{\perp})^2 (V_k^{\perp})^T \tilde{q}_k + \tilde{q}_k^T V_k \Sigma_k^2 V_k^T \tilde{q}_k. \end{split}$$
(69)

Observe that it is impossible for  $(V_k^\perp)^T \tilde{q}_k$  and  $V_k^T \tilde{q}_k$  to be the eigenvectors of  $(\Sigma_k^\perp)^2$  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  $e_{n-k}$  of  $\mathbb{R}^{n-k}$  and the k-th canonical vector  $e_k$  of  $\mathbb{R}^k$ , respectively; otherwise, we have  $\tilde{q}_k = v_n$  and  $\tilde{q}_k = v_k$  simultaneously, which are impossible as k < n. Therefore, from (69), (66) and (68), we obtain the strict inequality

$$\tilde{q}_{k}^{T} A^{T} A \tilde{q}_{k} > \|(V_{k}^{\perp})^{T} \tilde{q}_{k}\|^{2} \sigma_{n}^{2} + \|V_{k}^{T} \tilde{q}_{k}\|^{2} \sigma_{k}^{2} = (1 - \varepsilon_{k}^{2}) \sigma_{n}^{2} + \varepsilon_{k}^{2} \sigma_{k}^{2},$$

from which it follows that the lower bound of (63) holds. Similarly, from (69) and (66), (68) we obtain the upper bound of (63):

$$\tilde{q}_{k}^{T} A^{T} A \tilde{q}_{k} < \| (V_{k}^{\perp})^{T} \tilde{q}_{k} \|^{2} \| (\Sigma_{k}^{\perp})^{2} \| + \| V_{k}^{T} \tilde{q}_{k} \|^{2} \| \Sigma_{k}^{2} \| = (1 - \varepsilon_{k}^{2}) \sigma_{k+1}^{2} + \varepsilon_{k}^{2} \sigma_{1}^{2}.$$

From the lower bound of (63), we see that if  $\varepsilon_k$  satisfies  $\varepsilon_k^2 \sigma_k^2 \ge \sigma_{k+1}^2$ , i.e.,  $\varepsilon_k \ge \frac{\sigma_{k+1}}{\sigma_k}$ , then  $\sqrt{\tilde{q}_k^T A^T A \tilde{q}_k} > \sigma_{k+1}$ , i.e., (64) holds.

From (15), we obtain  $B_k^T B_k = Q_k^T A^T A Q_k$ . Note that  $(\theta_k^{(k)})^2$  is the smallest eigenvalue of the symmetric positive definite matrix  $B_k^T B_k$ . Therefore, we have

$$(\theta_k^{(k)})^2 = \min_{\|c\|=1} c^T Q_k^T A^T A Q_k c = \min_{q \in \mathcal{V}^R, \|q\|=1} q^T A^T A q = \hat{q}_k^T A^T A \hat{q}_k, \tag{70}$$

where  $\hat{q}_k$  is, in fact, the Ritz vector of  $A^TA$  from  $\mathcal{V}_k^R$  corresponding to the smallest Ritz value  $(\theta_k^{(k)})^2$ . Therefore, for  $\tilde{q}_k$  defined in Theorem 4 we have

$$\theta_k^{(k)} \leq \sqrt{\tilde{q}_k^T A^T A \tilde{q}_k},$$

from which it follows from (63) that  $(\theta_k^{(k)})^2 < (1 - \varepsilon_k^2)\sigma_{k+1}^2 + \varepsilon_k^2\sigma_1^2$ . As a result, for any  $\delta > 0$ , we can choose  $\varepsilon_k \geq 0$  such that

$$(\theta_k^{(k)})^2 < (1 - \varepsilon_k^2)\sigma_{k+1}^2 + \varepsilon_k^2\sigma_1^2 \le (1 + \delta)\sigma_{k+1}^2,$$

i.e., (65) holds, solving which for  $\varepsilon_k^2$  gives  $\varepsilon_k^2 \leq \frac{\delta}{(\frac{\sigma_1}{\sigma_{k+1}})^2 - 1}$ .

Remark 8 We analyze  $\theta_k^{(k)}$  when  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$ . In the sense of min in (70),  $\hat{q}_k \in \mathcal{V}_k^R$  is the optimal vector that extracts the least information from  $\mathcal{V}_k$  and the richest information from  $span\{V_k^{\perp}\}$ . From Theorem 4, since  $\mathcal{V}_k$  is the orthogonal complement of  $span\{V_k^{\perp}\}$ , we know that  $\tilde{q}_k \in \mathcal{V}_k^R$  has the largest acute angle with  $\mathcal{V}_k$ , that is, it contains the least information from  $\mathcal{V}_k$  and the richest information from  $span\{V_k^{\perp}\}$ . Therefore,  $\hat{q}_k$  and  $\tilde{q}_k$  have a similar optimality, so that we have

$$\theta_k^{(k)} \approx \sqrt{\tilde{q}_k^T A^T A \tilde{q}_k}. (71)$$

Combining this estimate with (64), we may have  $\theta_k^{(k)} > \sigma_{k+1}$  when  $\varepsilon_k \ge \frac{\sigma_{k+1}}{\sigma_k}$ .

Remark 9 We inspect the condition  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$  for (64) and get insight into whether or not the true  $\varepsilon_k$  resulting from the three kinds of ill-posed problems satisfies it. For severely ill-posed problems, the lower bound  $\frac{\sigma_{k+1}}{\sigma_k}$  is basically  $\rho^{-1}$ ; for moderately ill-posed problems with  $\alpha > 1$ , the bound increases with increasing  $k \le k_0$ , and it cannot be close to one provided that  $\alpha > 1$  suitably or  $k_0$  not big; for mildly ill-posed problems with  $\alpha$  < 1, the bound increases faster than it does for moderately ill-posed problems, and it may well approach one for  $k \leq k_0$ . Therefore, the condition for (64) requires that  $\|\sin\Theta(\mathscr{V}_k,\mathscr{V}_k^R)\|$  be not close to one for severely and moderately ill-posed problems, but  $\|\sin\Theta(\mathscr{V}_k,\mathscr{V}_k^R)\|$  must be close to zero for mildly ill-posed problems. In view of (21) and  $\|\sin\Theta(\mathcal{V}_k,\mathcal{V}_k^R)\|^2 = 1 - \varepsilon_k^2$ , we have  $\|\Delta_k\|^2 = \frac{1 - \varepsilon_k^2}{\varepsilon_k^2}$ . Thus, the condition  $\varepsilon_k \ge \frac{\sigma_{k+1}}{\sigma_k}$  for (64) amounts to requiring that  $||\Delta_k||$  be at most modest and cannot be large for severely and moderately ill-posed problems but it must be fairly small for mildly ill-posed problems. Unfortunately, Theorems 1–3 and the remarks followed indicate that  $\|\Delta_k\|$  increases with k increasing and is generally large for a mildly ill-posed problem, while it increases slowly with  $k \le k_0$  for a moderately ill-posed problem with  $\alpha > 1$  suitably, and by (49) it 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, because the actual  $\|\Delta_k\|$  can hardly be small and is generally large, the true  $\varepsilon_k$  is small and may well be close to zero, so that the condition  $\varepsilon_k \ge \frac{\sigma_{k+1}}{\sigma_k}$  generally fails to meet as k increases, while it is satisfied for severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably.

Remark 10 (65) shows that there is at least one  $\theta_k^{(k)} \leq \sigma_{k+1}$  if  $\|\sin\Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  is sufficiently close to one since we can choose  $\delta$  small enough such that  $(1+\delta)^{1/2}\sigma_{k+1}$  is close to  $\sigma_{k+1}$  arbitrarily. As we have shown,  $\|\sin\Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  cannot be close to one for severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably, but it is generally so for mildly ill-posed problems. This means that for some  $k \leq k_0$  it is very likely that  $\theta_k^{(k)} \leq \sigma_{k+1}$  for mildly ill-posed problems.

We must be aware that our above analysis on  $\theta_k^{(k)} > \sigma_{k+1}$  is not rigorous because we cannot quantify *how small*  $\sqrt{\tilde{q}_k^T A^T A \tilde{q}_k} - \theta_k^{(k)}$  is. From  $\theta_k^{(k)} \le \sqrt{\tilde{q}_k^T A^T A \tilde{q}_k}$ , it is apparent that the condition  $\varepsilon_k \ge \frac{\sigma_{k+1}}{\sigma_k}$  may not be sufficient for  $\theta_k^{(k)} > \sigma_{k+1}$ . We delay our detailed and rigorous analysis to Section 4.

Theorems 1–3 establish necessary background for answering the fundamental concern by Björck and Eldén, and their proof approaches also provide key ingredients for some of the later results. We now present the following results, which will play a central role in our later analysis.

**Theorem 5** Assume that the discrete Picard condition (7) is satisfied, let  $\Delta_k \in \mathbb{R}^{(n-k)\times k}$  be defined as (30) and  $L_j^{(k)}(0)$  and  $L_{k_1}^{(k)}(0)$  defined as (25), and write  $\Delta_k = (\delta_1, \delta_2, \dots, \delta_k)$ . Then for severely ill-posed problems and  $k = 1, 2, \dots, n-1$  we have

$$\|\delta_j\| \le \frac{\sigma_{k+1}}{\sigma_j} \frac{|u_{k+1}^T b|}{|u_i^T b|} \left(1 + \mathcal{O}(\rho^{-2})\right) |L_j^{(k)}(0)|, \ k > 1, \ j = 1, 2, \dots, k,$$
 (72)

$$\|\delta_1\| \le \frac{\sigma_2}{\sigma_1} \frac{|u_2^T b|}{|u_1^T b|} \left( 1 + \mathcal{O}(\rho^{-2}) \right) |, \ k = 1$$
 (73)

and

$$\|\Sigma_{k}\Delta_{k}^{T}\| \leq \begin{cases} \sigma_{k+1} \frac{|u_{k+1}^{T}b|}{|u_{k}^{T}b|} \left(1 + \mathcal{O}(\rho^{-2})\right) & \text{for } 1 \leq k \leq k_{0}, \\ \sigma_{k+1} \sqrt{k - k_{0} + 1} \left(1 + \mathcal{O}(\rho^{-2})\right) & \text{for } k_{0} < k \leq n - 1; \end{cases}$$
(74)

for moderately or mild ill-posed problems with the singular values  $\sigma_j = \zeta j^{-\alpha}$  and  $\zeta$  a positive constant we have

$$\|\delta_j\| \le \frac{\sigma_k}{\sigma_j} \frac{|u_{k+1}^T b|}{|u_i^T b|} \sqrt{\frac{k}{2\alpha - 1}} |L_j^{(k)}(0)|, \ k > 1, \ j = 1, 2, \dots, k, \tag{75}$$

$$\|\delta_1\| \le \frac{|u_2^T b|}{|u_1^T b|} \sqrt{\frac{1}{2\alpha - 1}}, \ k = 1$$
 (76)

and

$$\|\Sigma_{k}\Delta_{k}^{T}\| \leq \begin{cases} \sigma_{1} \frac{|u_{2}^{T}b|}{|u_{k}^{T}b|} \sqrt{\frac{1}{2\alpha-1}} & for \ k=1, \\ \sigma_{k} \frac{|u_{k+1}^{T}b|}{|u_{k}^{T}b|} \sqrt{\frac{k^{2}}{4\alpha^{2}-1} + \frac{k}{2\alpha-1}} |L_{k_{1}}^{(k)}(0)| & for \ 1 < k \leq k_{0}, \\ \sigma_{k} \sqrt{\frac{kk_{0}}{4\alpha^{2}-1} + \frac{k(k-k_{0}+1)}{2\alpha-1}} |L_{k_{1}}^{(k)}(0)| & for \ k_{0} < k \leq n-1. \end{cases}$$

$$(77)$$

*Proof.* From (30) and (35), for j = 1, 2, ..., k and k > 1 we have

$$\|\delta_j\|^2 \le |L_j^{(k)}(0)|^2 \sum_{i=k+1}^n \frac{\sigma_i^2}{\sigma_j^2} \frac{|u_i^T b|^2}{|u_j^T b|^2}$$
(78)

and from (42), for k = 1 we have

$$\|\delta_1\|^2 = \sum_{i=2}^n \frac{\sigma_i^2}{\sigma_1^2} \frac{|u_i^T b|^2}{|u_i^T b|^2}.$$
 (79)

For severely ill-posed problems, k = 1, 2, ..., n-1 and j = 1, 2, ..., k, from (41) we obtain

$$\begin{split} \sum_{i=k+1}^n \frac{\sigma_i^2}{\sigma_j^2} \frac{|u_i^T b|^2}{|u_j^T b|^2} &= \frac{1}{\sigma_j^2 |u_j^T b|^2} \sum_{i=k+1}^n \sigma_i^2 |u_i^T b|^2 \\ &\leq \frac{\sigma_{k+1}^2}{\sigma_i^2} \frac{|u_{k+1}^T b|^2}{|u_j^T b|^2} \left(1 + \mathcal{O}(\rho^{-2})\right). \end{split}$$

For moderately or mildly ill-posed problems, k = 1, 2, ..., n - 1 and j = 1, 2, ..., k, from (54) we obtain

$$\begin{split} \sum_{i=k+1}^{n} \frac{\sigma_{i}^{2}}{\sigma_{j}^{2}} \frac{|u_{i}^{T}b|^{2}}{|u_{j}^{T}b|^{2}} &= \frac{1}{\sigma_{j}^{2} |u_{j}^{T}b|^{2}} \sum_{i=k+1}^{n} \sigma_{i}^{2} |u_{i}^{T}b|^{2} \\ &\leq \frac{\sigma_{k}^{2}}{\sigma_{j}^{2}} \frac{|u_{k+1}^{T}b|^{2}}{|u_{j}^{T}b|^{2}} \frac{k}{2\alpha - 1}. \end{split}$$

Combining the above with (78), (47) and  $(1 + \mathcal{O}(\rho^{-2})) |L_{k_1}^{(k)}(0)| = 1 + \mathcal{O}(\rho^{-2})$ ,  $k = 2, 3, \ldots, n-1$ , we obtain (72), while (75) follows from the above and (78) directly. For k = 1, from (79) and the above we get (73) and (76), respectively.

By (36), for k > 1 we have

$$|\Delta_k \Sigma_k| \leq |L_{k_1}^{(k)}(0)| \left| (\sigma_{k+1} u_{k+1}^T b, \sigma_{k+2} u_{k+2}^T b, \dots, \sigma_n u_n^T b)^T \left( \frac{1}{u_1^T b}, \frac{1}{u_2^T b}, \dots, \frac{1}{u_k^T b} \right) \right|.$$

Therefore, we get

$$\|\Sigma_{k}\Delta_{k}^{T}\| = \|\Delta_{k}\Sigma_{k}\| \le \||\Delta_{k}\Sigma_{k}\|\|$$

$$\le |L_{k_{1}}^{(k)}(0)| \left(\sum_{j=k+1}^{n} \sigma_{j}^{2} |u_{j}^{T}b|^{2}\right)^{1/2} \left(\sum_{j=1}^{k} \frac{1}{|u_{j}^{T}b|^{2}}\right)^{1/2}.$$
(80)

By (42), for k = 1 we have

$$\|\Delta_1 \Sigma_1\| = \left(\sum_{j=2}^n \sigma_j^2 |u_j^T b|^2\right)^{1/2} \frac{1}{|u_1^T b|}.$$

We have derived the bounds (41) and (54) for  $\left(\sum_{j=k+1}^n \sigma_j^2 |u_j^T b|^2\right)^{1/2}$  for severely and moderately or mildly ill-posed problems, respectively, from which we obtain (74) and (77) for k=1. In order to bound  $\|\Sigma_k \Delta_k^T\|$  for k>1, we need to estimate  $\left(\sum_{j=1}^k \frac{1}{|u_j^T b|^2}\right)^{1/2}$ . We next carry out this task for severely and moderately or mildly ill-posed problems, respectively, for each kind of which we consider the cases of  $k \leq k_0$  and  $k > k_0$  separately.

Case of  $k \le k_0$  for severely ill-posed problems: From the discrete Picard condition (7) and (38), we obtain

$$\begin{split} \sum_{j=1}^k \frac{1}{|u_j^T b|^2} &= \frac{1}{|u_k^T b|^2} \sum_{j=1}^k \frac{|u_k^T b|^2}{|u_j^T b|^2} = \frac{1}{|u_k^T b|^2} \left( 1 + \mathcal{O}\left(\sum_{j=1}^{k-1} \rho^{2(j-k)(1+\beta)}\right) \right) \\ &= \frac{1}{|u_k^T b|^2} \left( 1 + \mathcal{O}(\rho^{-2(1+\beta)}) \right). \end{split}$$

Case of  $k > k_0$  for severely ill-posed problems: From (38) and (39), we obtain

$$\begin{split} \sum_{j=1}^k \frac{1}{|u_j^T b|^2} &= \frac{1}{|u_k^T b|^2} \left( \sum_{j=1}^{k_0} \frac{|u_k^T b|^2}{|u_j^T b|^2} + \sum_{j=k_0+1}^k \frac{|u_k^T b|^2}{|u_j^T b|^2} \right) \\ &= \frac{1}{|u_k^T b|^2} \left( 1 + \mathcal{O}\left( \sum_{j=1}^{k_0-1} \rho^{2(j-k_0)(1+\beta)} \right) + k - k_0 \right) \\ &= \frac{1}{|u_k^T b|^2} \left( 1 + \mathcal{O}(\rho^{-2(1+\beta)}) + k - k_0 \right). \end{split}$$

Substituting the above two relations for the two cases into (80) and combining them with (41) and (47), we get (74).

Case of  $k \le k_0$  for moderately or mildly ill-posed problems: From (38) we have

$$\begin{split} \sum_{j=1}^k \frac{1}{|u_j^T b|^2} &= \frac{1}{|u_k^T b|^2} \sum_{j=1}^k \frac{|u_k^T b|^2}{|u_j^T b|^2} = \frac{1}{|u_k^T b|^2} \sum_{j=1}^k \left(\frac{j}{k}\right)^{2\alpha(1+\beta)} \\ &< \frac{1}{|u_k^T b|^2} \sum_{j=1}^k \left(\frac{j}{k}\right)^{2\alpha} = \frac{1}{|u_k^T b|^2} k \sum_{j=1}^k \frac{1}{k} \left(\frac{j}{k}\right)^{2\alpha} \\ &< \frac{1}{|u_k^T b|^2} \left(k \int_0^1 x^{2\alpha} dx + 1\right) = \frac{1}{|u_k^T b|^2} \left(\frac{k}{2\alpha + 1} + 1\right). \end{split}$$

Case of  $k > k_0$  for moderately or mildly ill-posed problems: From (38) and (39) we have

$$\begin{split} \sum_{j=1}^{k} \frac{1}{|u_{j}^{T}b|^{2}} &= \frac{1}{|u_{k}^{T}b|^{2}} \left( \sum_{j=1}^{k_{0}} \frac{|u_{k}^{T}b|^{2}}{|u_{j}^{T}b|^{2}} + \sum_{j=k_{0}+1}^{k} \frac{|u_{k}^{T}b|^{2}}{|u_{j}^{T}b|^{2}} \right) \\ &= \frac{1}{|u_{k}^{T}b|^{2}} \left( \sum_{j=1}^{k_{0}} \left( \frac{j}{k_{0}} \right)^{2\alpha(1+\beta)} + k - k_{0} \right) \\ &< \frac{1}{|u_{k}^{T}b|^{2}} \left( \sum_{j=1}^{k_{0}} \left( \frac{j}{k_{0}} \right)^{2\alpha} + k - k_{0} \right) \\ &\leq \frac{1}{|u_{k}^{T}b|^{2}} \left( \frac{k_{0}}{2\alpha+1} + 1 + k - k_{0} \right). \end{split}$$

Substituting the above two bounds for the two cases into (80) and combining them with (54), we get (77).  $\Box$ 

(74) and (77) indicate that  $\|\Sigma_k \Delta_k^T\|$  decays swiftly as k increases. As has been seen, we must take some cares to accurately bound  $\|\Sigma_k \Delta_k^T\|$ . Indeed, for  $1 < k \le k_0$ , if we had simply estimated it by

$$\|\Sigma_k \Delta_k^T\| \le \|\Sigma_k\| \|\Delta_k^T\| = \sigma_1 \|\Delta_k\|, \tag{81}$$

we would have obtained a bound, which not only does not decay but also increases for moderately and mildly ill-posed problems as *k* increases. Such bound is useless to precisely analyze the regularization of LSQR for ill-posed problems and makes us impossible to get those predictively accurate results to be presented in Sections 4–5.

## 4 The rank k approximation $P_{k+1}B_kQ_k^T$ to A, the Ritz values $\theta_i^{(k)}$ and the regularization of LSQR

Making use of Theorems 1–5, we are able to solve those key problems stated before Theorem 1 and give definitive answers to the fundamental concern by Björck and Eldén, proving that LSQR has the full regularization for severely or moderately illposed problems with  $\rho > 1$  or  $\alpha > 1$  suitably and it, in general, has only the partial regularization for mildly ill-posed problems.

Define

$$\gamma_k = \|A - P_{k+1} B_k Q_k^T \|, \tag{82}$$

which measures the accuracy of the rank k approximation  $P_{k+1}B_kQ_k^T$  to A generated by Lanczos bidiagonalization. Recall (17) and the comments followed. It is known that the full or partial regularization of LSQR uniquely depends on whether or not  $\gamma_k \approx \sigma_{k+1}$  holds, where we will make the precise meaning ' $\approx$ ' clear by introducing the definition of near best rank k approximation to A, and on whether or not the k Ritz values  $\theta_i^{(k)}$  approximate the k large singular values  $\sigma_i$  of A in natural order for  $k = 1, 2, \ldots, k_0$ . If both of them hold, LSQR has the full regularization; if either of them is not satisfied, LSQR has only the partial regularization.

### 4.1 Accuracy of the rank k approximation $P_{k+1}B_kQ_k^T$ to A

We first present one of the main results in this paper.

**Theorem 6** Assume that the discrete Picard condition (7) is satisfied. Then for k = 1, 2, ..., n-1 we have

$$\sigma_{k+1} \le \gamma_k \le \sqrt{1 + \eta_k^2} \sigma_{k+1} \tag{83}$$

with

$$\eta_{k} \leq \begin{cases}
\xi_{k} \frac{|u_{k+1}^{T}b|}{|u_{k}^{T}b|} \left(1 + \mathcal{O}(\rho^{-2})\right) & \text{for } 1 \leq k \leq k_{0}, \\
\xi_{k} \sqrt{k - k_{0} + 1} \left(1 + \mathcal{O}(\rho^{-2})\right) & \text{for } k_{0} < k \leq n - 1
\end{cases}$$
(84)

for severely ill-posed problems and

$$\eta_{k} \leq \begin{cases}
\xi_{1} \frac{\sigma_{1}}{\sigma_{2}} \frac{|u_{1}^{T}b|}{|u_{1}^{T}b|} \sqrt{\frac{1}{2\alpha-1}} & for \ k = 1, \\
\xi_{k} \frac{\sigma_{k}}{\sigma_{k+1}} \frac{|u_{k+1}^{T}b|}{|u_{k}^{T}b|} \sqrt{\frac{k^{2}}{4\alpha^{2}-1} + \frac{k}{2\alpha-1}} |L_{k_{1}}^{(k)}(0)| & for \ 1 < k \leq k_{0}, \\
\xi_{k} \frac{\sigma_{k}}{\sigma_{k+1}} \sqrt{\frac{kk_{0}}{4\alpha^{2}-1} + \frac{k(k-k_{0}+1)}{2\alpha-1}} |L_{k_{1}}^{(k)}(0)| & for \ k_{0} < k \leq n-1
\end{cases}$$
(85)

for moderately or mildly ill-posed problems with  $\sigma_j = \zeta j^{-\alpha}$ , j = 1, 2, ..., n, where  $\xi_k = \sqrt{\left(\frac{\|\Delta_k\|}{1+\|\Delta_k\|^2}\right)^2 + 1}$  for  $\|\Delta_k\| < 1$  and  $\xi_k \leq \frac{\sqrt{5}}{2}$  for  $\|\Delta_k\| \geq 1$ .

*Proof.* Since  $A_k$  is the best rank k approximation to A with respect to the 2-norm and  $||A - A_k|| = \sigma_{k+1}$ , the lower bound in (83) holds. Next we prove the upper bound. From (12), we obtain

$$\gamma_k = \|A - P_{k+1} B_k Q_k^T\| = \|A - A Q_k Q_k^T\| = \|A(I - Q_k Q_k^T)\|. \tag{86}$$

From Algorithm 1, (29), (31) and (32), we obtain

$$\mathcal{Y}_{k}^{R} = \mathcal{K}_{k}(A^{T}A, A^{T}b) = span\{Q_{k}\} = span\{\hat{Z}_{k}\}$$

with  $Q_k$  and  $\hat{Z}_k$  being orthonormal, and the orthogonal projector onto  $\mathcal{V}_k^R$  is thus

$$Q_k Q_k^T = \hat{Z}_k \hat{Z}_k^T. \tag{87}$$

Keep in mind that  $A_k = U_k \Sigma_k V_k^T$ . It is direct to justify that  $(U_k \Sigma_k V_k^T)^T (A - U_k \Sigma_k V_k^T) = \mathbf{0}$  for  $k = 1, 2, \dots, n-1$ . Therefore, exploiting this and noting that  $\|I - \hat{Z}_k \hat{Z}_k^T\| = 1$  and  $V_k^T V_k^T = \mathbf{0}$  for  $k = 1, 2, \dots, n-1$ , we get from (86), (87) and (32) that

$$\gamma_{k}^{2} = \|(A - U_{k} \Sigma_{k} V_{k}^{T} + U_{k} \Sigma_{k} V_{k}^{T})(I - \hat{Z}_{k} \hat{Z}_{k}^{T})\|^{2} \\
= \max_{\|y\|=1} \|(A - U_{k} \Sigma_{k} V_{k}^{T} + U_{k} \Sigma_{k} V_{k}^{T})(I - \hat{Z}_{k} \hat{Z}_{k}^{T})y\|^{2} \\
= \max_{\|y\|=1} \|(A - U_{k} \Sigma_{k} V_{k}^{T})(I - \hat{Z}_{k} \hat{Z}_{k}^{T})y + U_{k} \Sigma_{k} V_{k}^{T}(I - \hat{Z}_{k} \hat{Z}_{k}^{T})y\|^{2} \\
= \max_{\|y\|=1} (\|(A - U_{k} \Sigma_{k} V_{k}^{T})(I - \hat{Z}_{k} \hat{Z}_{k}^{T})y\|^{2} + \|U_{k} \Sigma_{k} V_{k}^{T}(I - \hat{Z}_{k} \hat{Z}_{k}^{T})y\|^{2}) \\
\leq \|(A - U_{k} \Sigma_{k} V_{k}^{T})(I - \hat{Z}_{k} \hat{Z}_{k}^{T})\|^{2} + \|U_{k} \Sigma_{k} V_{k}^{T}(I - \hat{Z}_{k} \hat{Z}_{k}^{T})\|^{2} \\
\leq \sigma_{k+1}^{2} + \|\Sigma_{k} V_{k}^{T}(I - \hat{Z}_{k} \hat{Z}_{k}^{T})\|^{2} \\
\leq \sigma_{k+1}^{2} + \|\Sigma_{k} V_{k}^{T}(I - \hat{Z}_{k} \hat{Z}_{k}^{T})\|^{2} \\
= \sigma_{k+1}^{2} + \|\Sigma_{k} (V_{k}^{T} - (I + \Delta_{k}^{T} \Delta_{k})^{-1}(V_{k} + V_{k}^{\perp} \Delta_{k})^{T})\|^{2} \\
= \sigma_{k+1}^{2} + \|\Sigma_{k} (I + \Delta_{k}^{T} \Delta_{k})^{-1} \left((I + \Delta_{k}^{T} \Delta_{k})V_{k}^{T} - \left(V_{k} + V_{k}^{\perp} \Delta_{k}\right)^{T}\right)\|^{2} \\
= \sigma_{k+1}^{2} + \|\Sigma_{k} (I + \Delta_{k}^{T} \Delta_{k})^{-1} \left(\Delta_{k}^{T} \Delta_{k} V_{k}^{T} - \Delta_{k}^{T}(V_{k}^{\perp})^{T}\right)\|^{2} \\
= \sigma_{k+1}^{2} + \|\Sigma_{k} (I + \Delta_{k}^{T} \Delta_{k})^{-1} \Delta_{k}^{T} \Delta_{k} V_{k}^{T} - \Sigma_{k} (I + \Delta_{k}^{T} \Delta_{k})^{-1} \Delta_{k}^{T}(V_{k}^{\perp})^{T}\|^{2} \\
\leq \sigma_{k+1}^{2} + \|\Sigma_{k} (I + \Delta_{k}^{T} \Delta_{k})^{-1} \Delta_{k}^{T} \Delta_{k} V_{k}^{T} - \Sigma_{k} (I + \Delta_{k}^{T} \Delta_{k})^{-1} \Delta_{k}^{T}(V_{k}^{\perp})^{T}\|^{2} \\
\leq \sigma_{k+1}^{2} + \|\Sigma_{k} (I + \Delta_{k}^{T} \Delta_{k})^{-1} \Delta_{k}^{T} \Delta_{k} \|^{2} + \|\Sigma_{k} (I + \Delta_{k}^{T} \Delta_{k})^{-1} \Delta_{k}^{T} \|^{2} \\
\leq \sigma_{k+1}^{2} + \varepsilon_{k}^{2}, \tag{89}$$

where the last inequality follows by using  $V_k^T V_k^{\perp} = \mathbf{0}$  and the definition of the induced matrix 2-norm to amplify the second term in (88).

We estimate  $\varepsilon_k$  accurately below. To this end, we need to use two key identities and some results related. By the SVD of  $\Delta_k$ , it is direct to justify that

$$(I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T \Delta_k = \Delta_k^T \Delta_k (I + \Delta_k^T \Delta_k)^{-1}$$
(90)

and

$$(I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T = \Delta_k^T (I + \Delta_k \Delta_k^T)^{-1}. \tag{91}$$

Define the function  $f(\lambda) = \frac{\lambda}{1+\lambda^2}$  with  $\lambda \in [0,\infty)$ . Since the derivative  $f'(\lambda) = \frac{1-\lambda^2}{(1+\lambda^2)^2}$ ,  $f(\lambda)$  is monotonically increasing for  $\lambda \in [0,1]$  and decreasing for  $\lambda \in [1,\infty)$ , and the maximum of  $f(\lambda)$  over  $\lambda \in [0,\infty)$  is  $\frac{1}{2}$ , which attains at  $\lambda = 1$ . Based on these properties and exploiting the SVD of  $\Delta_k$ , for the matrix 2-norm we get

$$\|\Delta_k (I + \Delta_k^T \Delta_k)^{-1}\| = \frac{\|\Delta_k\|}{1 + \|\Delta_k\|^2}$$
(92)

for  $||\Delta_k|| < 1$  and

$$\|\Delta_k(I + \Delta_k^T \Delta_k)^{-1}\| \le \frac{1}{2} \tag{93}$$

for  $||\Delta_k|| \ge 1$  (Note: in this case, since  $\Delta_k$  may have at least one singular value smaller than one, we do not have an expression like (92)). It then follows from (89), (92), (93) and  $||(1 + \Delta_k \Delta_k^T)^{-1}|| \le 1$  that

$$\varepsilon_{k}^{2} = \|\Sigma_{k} \Delta_{k}^{T} \Delta_{k} (I + \Delta_{k}^{T} \Delta_{k})^{-1} \|^{2} + \|\Sigma_{k} \Delta_{k}^{T} (I + \Delta_{k} \Delta_{k}^{T})^{-1} \|^{2} 
\leq \|\Sigma_{k} \Delta_{k}^{T} \|^{2} \|\Delta_{k} (I + \Delta_{k}^{T} \Delta_{k})^{-1} \|^{2} + \|\Sigma_{k} \Delta_{k}^{T} \|^{2} \|(1 + \Delta_{k} \Delta_{k}^{T})^{-1} \|^{2} 
\leq \|\Sigma_{k} \Delta_{k}^{T} \|^{2} (\|\Delta_{k} (I + \Delta_{k}^{T} \Delta_{k})^{-1} \|^{2} + 1) 
= \|\Sigma_{k} \Delta_{k}^{T} \|^{2} \left( \left( \frac{\|\Delta_{k} \|}{1 + \|\Delta_{k} \|^{2}} \right)^{2} + 1 \right) = \xi_{k}^{2} \|\Sigma_{k} \Delta_{k}^{T} \|^{2}$$
(94)

for  $||\Delta_k|| < 1$  and

$$\varepsilon_k \leq \|\Sigma_k \Delta_k^T\| \sqrt{\|\Delta_k (I + \Delta_k^T \Delta_k)^{-1}\|^2 + 1} = \xi_k \|\Sigma_k \Delta_k^T\| \leq \frac{\sqrt{5}}{2} \|\Sigma_k \Delta_k^T\|$$

for  $\|\Delta_k\| \ge 1$ . Replace  $\|\Sigma_k \Delta_k^T\|$  by its bounds (74) and (77) in the above, insert the resulting bounds for  $\varepsilon_k$  into (89), and let  $\varepsilon_k = \eta_k \sigma_{k+1}$ . Then we obtain the upper bound in (83) with  $\eta_k$  satisfying (84) and (85) for severely and moderately or mildly ill-posed problems, respectively.

Note from (38) that

$$\frac{|u_{k+1}^T b|}{|u_k^T b|} = \frac{\sigma_{k+1}^{1+\beta}}{\sigma_k^{1+\beta}}, \ k \le k_0.$$

Therefore, for the right-hand side of (85) and  $k \le k_0$  we have

$$\frac{\sigma_k}{\sigma_{k+1}} \frac{|u_{k+1}^T b|}{|u_k^T b|} = \left(\frac{\sigma_{k+1}}{\sigma_k}\right)^{\beta} < 1.$$

Remark 11 For severely ill-posed problems, from (49), (50) and the definition of  $\xi_k$  we know that

$$\xi_k(1 + \mathcal{O}(\rho^{-2})) = 1 + \mathcal{O}(\rho^{-2})$$

for both  $k \le k_0$  and  $k > k_0$ . Therefore, from (84) and (38), for  $k \le k_0$  we have

$$\eta_k \le \xi_k \frac{|u_{k+1}^T b|}{|u_k^T b|} \left( 1 + \mathscr{O}(\rho^{-2}) \right) = \frac{|u_{k+1}^T b|}{|u_k^T b|} = \frac{\sigma_{k+1}^{1+\beta}}{\sigma_k^{1+\beta}} = \mathscr{O}(\rho^{-1-\beta}) < 1 \tag{95}$$

by ignoring the smaller term  $\mathcal{O}(\rho^{-1-\beta})\mathcal{O}(\rho^{-2}) = \mathcal{O}(\rho^{-3-\beta})$ , and for  $k > k_0$  we have

$$\eta_k \le \xi_k \sqrt{k - k_0 + 1} \left( 1 + \mathcal{O}(\rho^{-2}) \right) = \sqrt{k - k_0 + 1}$$
 (96)

by ignoring the smaller term  $\sqrt{k-k_0+1}\mathcal{O}(\rho^{-2})$ , which increases slowly with k.

Remark 12 For the moderately or mildly ill-posed problems with  $\sigma_j = \zeta j^{-\alpha}$ , from the derivation on  $\eta_k$  and its estimate (85), for  $k \le k_0$  we approximately have

$$\frac{\sigma_k}{\sigma_{k+1}} \|\Delta_k\| \le \eta_k \le \frac{\sqrt{5}}{2} \frac{\sigma_k}{\sigma_{k+1}} \|\Delta_k\|, \tag{97}$$

and for  $k > k_0$ , from (60) and (61) we approximately have

$$\eta_{k} < \frac{\sigma_{k}}{\sigma_{k+1}} \sqrt{\frac{kk_{0}}{4\alpha^{2} - 1} + \frac{k(k - k_{0} + 1)}{2\alpha - 1}} |L_{k_{1}}^{(k)}(0)| 
\sim \frac{k^{3/2} \sqrt{k_{0}}}{(2\alpha + 1)\sqrt{4\alpha^{2} - 1}} + \frac{k^{3/2} \sqrt{k - k_{0} + 1}}{(2\alpha + 1)\sqrt{2\alpha - 1}},$$
(98)

which increases faster than the right-hand side of (96) with respect to k.

Remark 13 From (83), (84) and (95), for severely ill-posed problems we have

$$1 < \sqrt{1 + \eta_k^2} < 1 + \frac{1}{2}\eta_k^2 \le 1 + \frac{1}{2}\frac{\sigma_{k+1}^{2(1+\beta)}}{\sigma_k^{2(1+\beta)}} \sim 1 + \frac{1}{2}\rho^{-2(1+\beta)},$$

and  $\gamma_k$  is an accurate approximation to  $\sigma_{k+1}$  for  $k \leq k_0$  and marginally less accurate for  $k > k_0$ . Thus, the rank k approximation  $P_{k+1}B_kQ_k^T$  is as accurate as the best rank k approximation  $A_k$  within the factor  $\sqrt{1+\eta_k^2}\approx 1$  for  $k\leq k_0$  and  $\rho>1$  suitably. For moderately ill-posed problems,  $\gamma_k$  is still an excellent approximation to  $\sigma_{k+1}$ , and the rank k approximation  $P_{k+1}B_kQ_k^T$  is almost as accurate as the best rank k approximation  $A_k$  for  $k\leq k_0$ . Therefore,  $P_{k+1}B_kQ_k^T$  plays the same role as  $A_k$  for these two kinds of ill-posed problems and  $k\leq k_0$ , it is known from the clarification in Section 2 that LSQR may have the full regularization. We will, afterwards, deepen this theorem and derive more results, proving that LSQR must have the full regularization for these two kinds of problems provided that  $\rho>1$  and  $\alpha>1$  suitably.

For both severely and moderately ill-posed problems, we note that the situation is not so satisfying for increasing  $k > k_0$ . But at that time, a possibly big  $\eta_k$  does not do harm to our regularization purpose since we will prove that, provided that  $\rho > 1$  and  $\alpha > 1$  suitably, LSQR has the full regularization and has already found a best possible regularized solution at semi-convergence occurring at iteration  $k_0$ . If it is the case, we will simply stop performing it after semi-convergence.

Remark 14 For mildly ill-posed problems, the situation is fundamentally different. As clarified in Remark 7, we have  $\sqrt{\frac{k^2}{4\alpha^2-1}+\frac{k}{2\alpha-1}}>1$  and  $|L_{k_1}^{(k)}(0)|>1$  considerably as k increases up to  $k_0$  because of  $\frac{1}{2}<\alpha\leq 1$ , leading to  $\eta_k>1$  substantially. This means that  $\gamma_{k_0}$  is substantially bigger than  $\sigma_{k_0+1}$  and can well lie between  $\sigma_{k_0}$  and  $\sigma_1$ , so that the rank  $k_0$  approximation  $P_{k_0+1}B_{k_0}Q_{k_0}^T$  is much less accurate than the best rank  $k_0$  approximation  $A_{k_0}$  and LSQR has only the partial regularization.

Remark 15 There are several subtle treatments in the proof of Theorem 6, each of which turns out to be absolutely necessary. Ignoring or missing any one of them would be fatal and make us fail to obtain accurate estimates for  $\varepsilon_k$  defined by (89). The first is the treatment of  $\|U_k\Sigma_k V_k^T(I-\hat{Z}_k\hat{Z}_k^T)\|$ . By the definition of  $\|\sin\Theta(\mathscr{V}_k,\mathscr{V}_k^R)\|$ , if we had amplified it by

$$||U_k \Sigma_k V_k^T (I - \hat{Z}_k \hat{Z}_k^T)|| < ||\Sigma_k|| ||V_k^T (I - \hat{Z}_k \hat{Z}_k^T)|| = \sigma_1 ||\sin \Theta(\mathcal{Y}_k, \mathcal{Y}_k^R)||,$$

we would have obtained a too large overestimate, which is almost a fixed constant for severely ill-posed problems and  $k=1,2,\ldots,k_0$  and increases with  $k=1,2,\ldots,k_0$  for moderately and mildly ill-posed problems. Such rough estimates are useless to get a meaningful bound for  $\gamma_k$ . The second is the use of (90) and (91). The third is the extraction of  $\|\Sigma_k \Delta_k^T\|$  from (94) as a whole other than amplify it to  $\|\Sigma_k\|\|\Delta_k\| = \sigma_1\|\Delta_k\|$ . The fourth is accurate estimates for it; see (74) and (77) in Theorem 5. For example, without using (90) and (91), by (21) we would have no way but to obtain

$$\begin{split} & \varepsilon_k^2 \leq \|\Sigma_k\|^2 \|(I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T \Delta_k\|^2 + \|\Sigma_k\|^2 \|(I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T\|^2 \\ & = \sigma_1^2 \left( \frac{\|\Delta_k\|^2}{1 + \|\Delta_k\|^2} \right)^2 + \sigma_1^2 \|(I + \Delta_k^T \Delta_k)^{-1} \Delta_k^T\|^2 \\ & = \sigma_1^2 \|\sin\Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|^4 + \sigma_1^2 \|\Delta_k (I + \Delta_k^T \Delta_k)^{-1}\|^2. \end{split}$$

From (93) and the previous estimates for  $\|\Delta_k\|$ , such bound is too pessimistic and completely useless in our context, and it even does not decrease and could not be small as k increases, while our estimates for  $\varepsilon_k = \eta_k \sigma_{k+1}$  in Theorem 6 are much more accurate and decay swiftly as k increases, as indicated by (84) and (85).

In order to prove the full or partial regularization of LSQR for (1) completely and rigorously, besides Theorem 6, we need to introduce a precise definition of the near best rank k approximation  $P_{k+1}B_kQ_k^T$  to A. By definition (82), the rank k matrix  $P_{k+1}B_kQ_k^T$  is called a near best rank k approximation to A if it satisfies

$$\sigma_{k+1} \le \gamma_k < \sigma_k \text{ and } \gamma_k - \sigma_{k+1} < \sigma_k - \gamma_k, \text{ i.e., } \gamma_k < \frac{\sigma_k + \sigma_{k+1}}{2},$$
 (99)

that is,  $\gamma_k$  lies between  $\sigma_k$  and  $\sigma_{k+1}$  and is closer to  $\sigma_{k+1}$ . This definition is natural. We mention in passing that a near best rank k approximation to A from an ill-posed problem is much more stringent than it is for a matrix from a numerically rank-deficient problem where the large singular values are well separated from the small ones and there is a substantial gap between two groups of singular values.

Based on Theorem 6, for the severely and moderately or mildly ill-posed problems with the singular value models  $\sigma_k = \zeta \rho^{-k}$  and  $\sigma_k = \zeta k^{-\alpha}$ , we next derive the

sufficient conditions on  $\rho$  and  $\alpha$  that guarantee that  $P_{k+1}B_kQ_k^T$  is a near best rank k approximation to A for  $k=1,2,\ldots,k_0$ . We analyze if and how the sufficient conditions are satisfied for three kinds of ill-posed problems.

**Theorem 7** For a given (1), assume that the discrete Picard condition (7) is satisfied. Then, in the sense of (99),  $P_{k+1}B_kQ_k^T$  is a near best rank k approximation to A for  $k = 1, 2, ..., k_0$  if

$$\sqrt{1+\eta_k^2} < \frac{1}{2} \frac{\sigma_k}{\sigma_{k+1}} + \frac{1}{2}.$$
 (100)

For the severely ill-posed problems with  $\sigma_k = \zeta \rho^{-k}$  and the moderately or mildly ill-posed problems with  $\sigma_k = \zeta k^{-\alpha}$ ,  $P_{k+1}B_kQ_k^T$  is a near best rank k approximation to A for  $k = 1, 2, \ldots, k_0$  if  $\rho > 2$  and  $\alpha$  satisfies

$$2\sqrt{1+\eta_k^2} - 1 < \left(\frac{k_0 + 1}{k_0}\right)^{\alpha},\tag{101}$$

respectively.

*Proof.* By (83), we see that  $\gamma_k \leq \sqrt{1 + \eta_k^2} \sigma_{k+1}$ . Therefore,  $P_{k+1} B_k Q_k^T$  is a near best rank k approximation to A in the sense of (99) provided that

$$\sqrt{1+\eta_k^2}\sigma_{k+1}<\sigma_k$$

and

$$\sqrt{1+\eta_k^2}\sigma_{k+1}<\frac{\sigma_k+\sigma_{k+1}}{2},$$

from which (100) follows.

From (95), for the severely ill-posed problems with  $\sigma_k = \zeta \rho^{-k}$  and  $\rho > 1$  we have

$$\sqrt{1+\eta_k^2} < 1 + \frac{1}{2}\eta_k^2 \le 1 + \frac{1}{2}\rho^{-2(1+\beta)} < 1 + \rho^{-1}, \ k = 1, 2, \dots, k_0, \tag{102}$$

from which it follows that

$$\sqrt{1+\eta_k^2}\sigma_{k+1} < (1+\rho^{-1})\sigma_{k+1}. \tag{103}$$

Since  $\sigma_k/\sigma_{k+1} = \rho$ , (100) holds provided that

$$1 + \rho^{-1} < \frac{1}{2}\rho + \frac{1}{2},$$

i.e.,  $\rho^2 - \rho - 2 > 0$ , solving which for  $\rho$  we get  $\rho > 2$ . For the moderately or mildly ill-posed problems with  $\sigma_k = \zeta k^{-\alpha}$ , it is direct from (100) to get

$$2\sqrt{1+\eta_k^2}-1<\left(\frac{k+1}{k}\right)^{\alpha}.$$

Since  $\left(\frac{k+1}{k}\right)^{\alpha}$  decreases monotonically as k increases, its minimum over  $k = 1, 2, \dots, k_0$  is  $\left(\frac{k_0+1}{k_0}\right)^{\alpha}$ . Therefore, we obtain (101).

Remark 16 Given the noise level ||e||, the discrete Picard condition (7) and (8), from the bound (85) for  $\eta_k$ ,  $k = 1, 2, ..., k_0$ , we see that the bigger  $\alpha > 1$  is, the smaller  $k_0$  and  $\eta_k$  are. Therefore, there must be  $\alpha > 1$  such that (101) holds. Here we should remind that it is more suitable to regard the conditions on  $\rho$  and  $\alpha$  as an indication that  $\rho$  and  $\alpha$  must not be close to one other than precise requirements since we have used the bigger (102) and simplified models  $\sigma_k = \zeta \rho^{-k}$  and  $\sigma_k = \zeta k^{-\alpha}$ .

Remark 17 For the mildly ill-posed problems with  $\sigma_k = \zeta k^{-\alpha}$ , Theorem 3 has shown that  $\|\Delta_k\|$  is generally not small and can be arbitrarily large for  $k=1,2,\ldots,k_0$ . From (97), we see that the size of  $\eta_k$  is comparable to  $\|\Delta_k\|$ . Note that the right-hand side  $\left(\frac{k_0+1}{k_0}\right)^{\alpha} \leq 2$  for  $\frac{1}{2} < \alpha \leq 1$  and any  $k_0 \geq 1$ . Consequently, (101) cannot be met generally for mildly ill-posed problems. The rare possible exceptions are that  $k_0$  is only very few and  $\alpha$  is close to one since, in such case,  $\eta_k$  is not large for  $k=1,2,\ldots,k_0$ . So,  $P_{k+1}B_kQ_k^T$  is generally not a near best rank k approximation to  $k=1,2,\ldots,k_0$  for this kind of problem.

### 4.2 The approximation behavior of the Ritz values $\theta_i^{(k)}$

Starting with Theorem 6, we prove that, under certain sufficient conditions on  $\rho$  and  $\alpha$  for the severely and moderately ill-posed problems with the models  $\sigma_i = \zeta \rho^{-i}$  and  $\sigma_i = \zeta i^{-\alpha}$ , respectively, the k Ritz values  $\theta_i^{(k)}$  approximate the first k large singular values  $\sigma_i$  in natural order for  $k=1,2,\ldots,k_0$ , which means that no Ritz value smaller than  $\sigma_{k_0+1}$  appears. Combining this result with Theorem 7, we can draw the definitive conclusion that LSQR must have the full regularization for these two kinds of problems provided that  $\rho>1$  and  $\alpha>1$  suitably. On the other hand, we will show why LSQR generally has only the partial regularization for mildly ill-posed problems.

**Theorem 8** Assume that (1) is severely ill-posed with  $\sigma_i = \zeta \rho^{-i}$  and  $\rho > 1$  or moderately ill-posed with  $\sigma_i = \zeta i^{-\alpha}$  and  $\alpha > 1$ , and the discrete Picard condition (7) is satisfied. Let the Ritz values  $\theta_i^{(k)}$  be labeled as  $\theta_1^{(k)} > \theta_2^{(k)} > \cdots > \theta_k^{(k)}$ . Then

$$0 < \sigma_i - \theta_i^{(k)} \le \sqrt{1 + \eta_k^2} \sigma_{k+1}, \ i = 1, 2, \dots, k.$$
 (104)

If  $\rho \ge 1 + \sqrt{2}$  or  $\alpha > 1$  satisfies

$$1 + \sqrt{1 + \eta_k^2} < \left(\frac{k_0 + 1}{k_0}\right)^{\alpha}, \ k = 1, 2, \dots, k_0, \tag{105}$$

then the k Ritz values  $\theta_i^{(k)}$  strictly interlace the first large k+1 singular values of A and approximate the first k large ones in natural order for  $k=1,2,\ldots,k_0$ :

$$\sigma_{i+1} < \theta_i^{(k)} < \sigma_i, i = 1, 2, \dots, k,$$
 (106)

meaning that there is no Ritz value  $\theta_i^{(k)}$  smaller than  $\sigma_{k_0+1}$  for  $k=1,2,\ldots,k_0$ .

*Proof.* Note that for  $k=1,2,\ldots,k_0$  the  $\theta_i^{(k)}$ ,  $i=1,2,\ldots,k$  are just the nonzero singular values of  $P_{k+1}B_kQ_k^T$ , whose other n-k singular values are zeros. We write

$$A = P_{k+1}B_kQ_k^T + (A - P_{k+1}B_kQ_k^T)$$

with  $||A - P_{k+1}B_kQ_k^T|| = \gamma_k$  by definition (82). Then by the Mirsky's theorem of singular values [95, p.204, Thm 4.11], we have

$$|\sigma_i - \theta_i^{(k)}| \le \gamma_k \le \sqrt{1 + \eta_k^2} \sigma_{k+1}, \ i = 1, 2, \dots, k.$$
 (107)

Since the singular values of A are simple and b has components in all the left singular vectors  $u_1, u_2, \ldots, u_n$  of A, Lanczos bidiagonalization, i.e., Algorithm 1, can be run to completion, producing  $P_{n+1}$ ,  $Q_n$  and the lower bidiagonal  $B_n \in \mathbb{R}^{(n+1)\times n}$  such that

$$P^{T}AQ_{n} = \begin{pmatrix} B_{n} \\ \mathbf{0} \end{pmatrix} \tag{108}$$

with the  $m \times m$  matrix  $P = (P_{n+1}, \hat{P})$  and  $n \times n$  matrix  $Q_n$  orthogonal and all the  $\alpha_i$  and  $\beta_{i+1}$ , i = 1, 2, ..., n, of  $B_n$  being positive. Note that the singular values of  $B_k$ , k = 1, 2, ..., n, are all simple and that  $B_k$  consists of the first k columns of  $B_n$  with the last n - k zero rows deleted. Applying the Cauchy's *strict* interlacing theorem [95, p.198, Corollary 4.4] to the singular values of  $B_k$  and  $B_n$ , we have

$$\sigma_{n-k+i} < \theta_i^{(k)} < \sigma_i, \ i = 1, 2, \dots, k.$$
 (109)

Therefore, (107) becomes

$$0 < \sigma_i - \theta_i^{(k)} \le \gamma_k \le \sqrt{1 + \eta_k^2} \sigma_{k+1}, \ i = 1, 2, \dots, k, \tag{110}$$

which proves (104). That is, the  $\theta_i^{(k)}$  approximate  $\sigma_i$  from below for  $i=1,2,\ldots,k$  with the errors no more than  $\gamma_k \leq \sqrt{1+\eta_k^2}\sigma_{k+1}$ . For  $i=1,2,\ldots,k$ , notice that  $\rho^{-k+i} \leq 1$ . Then from (110), (102) and  $\sigma_i = \zeta \rho^{-i}$  we obtain

$$\begin{split} \theta_i^{(k)} &\geq \sigma_i - \gamma_k > \sigma_i - (1 + \rho^{-1})\sigma_{k+1} \\ &= \zeta \rho^{-i} - \zeta (1 + \rho^{-1})\rho^{-(k+1)} \\ &= \zeta \rho^{-(i+1)} (\rho - (1 + \rho^{-1})\rho^{-k+i}) \\ &\geq \zeta \rho^{-(i+1)} (\rho - \rho^{-1} - 1) \\ &\geq \zeta \rho^{-(i+1)} = \sigma_{i+1}, \end{split}$$

provided that  $\rho - \rho^{-1} \ge 2$ , solving which we get  $\rho \ge 1 + \sqrt{2}$ . Together with the upper bound of (109), we have proved (106).

For the moderately ill-posed problems with  $\sigma_i = \zeta i^{-\alpha}$ , i = 1, 2, ..., k and  $k = 1, 2, ..., k_0$ , we get

$$\begin{split} \theta_i^{(k)} &\geq \sigma_i - \gamma_k \geq \sigma_i - \sqrt{1 + \eta_k^2} \sigma_{k+1} \\ &= \zeta i^{-\alpha} - \zeta \sqrt{1 + \eta_k^2} (k+1)^{-\alpha} \\ &= \zeta (i+1)^{-\alpha} \left( \left( \frac{i+1}{i} \right)^{\alpha} - \sqrt{1 + \eta_k^2} \left( \frac{i+1}{k+1} \right)^{\alpha} \right) \\ &> \zeta (i+1)^{-\alpha} = \sigma_{i+1}, \end{split}$$

i.e., (106) holds, provided that  $\eta_k > 0$  and  $\alpha > 1$  are such that

$$\left(\frac{i+1}{i}\right)^{\alpha} - \sqrt{1+\eta_k^2} \left(\frac{i+1}{k+1}\right)^{\alpha} > 1,$$

which means that

$$\sqrt{1+\eta_k^2} < \left(\left(\frac{i+1}{i}\right)^{\alpha} - 1\right) \left(\frac{k+1}{i+1}\right)^{\alpha} = \left(\frac{k+1}{i}\right)^{\alpha} - \left(\frac{k+1}{i+1}\right)^{\alpha}, \ i = 1, 2, \dots, k.$$

It is easily justified that the above right-hand side monotonically decreases with respect to  $i=1,2,\ldots,k$ , whose minimum attains at i=k and equals  $\left(\frac{k+1}{k}\right)^{\alpha}-1$ . Furthermore, since  $\left(\frac{k+1}{k}\right)^{\alpha}-1$  decreases monotonically as k increases, its minimum over  $k=1,2,\ldots,k_0$  is  $\left(\frac{k_0+1}{k_0}\right)^{\alpha}-1$ , which is just the condition (105).

Remark 18 Similar to (101), there must be  $\alpha > 1$  such that (105) holds. Comparing Theorem 7 with Theorem 8, we find out that, as far as the severely or moderately illposed problems are concerned, for  $k = 1, 2, ..., k_0$  the near best rank approximation  $P_{k+1}B_kQ_k^T$  essentially means that the singular values  $\theta_i^{(k)}$  of  $B_k$  approximate the first k large singular values  $\sigma_i$  of A in natural order, provided that  $\rho > 1$  or  $\alpha > 1$  suitably.

*Remark 19* In terms of the above remarks, Theorems 6–8 show that LSQR has the full regularization for these two kinds of ill-posed problems with  $\rho > 1$  and  $\alpha > 1$  suitably and can obtain best possible regularized solutions  $x^{(k_0)}$  at semi-convergence.

For mildly ill-posed problems. We observe that the sufficient condition (105) for (106) is never met for this kind of problem because  $\left(\frac{k_0+1}{k_0}\right)^{\alpha} \leq 2$  for any  $k_0$  and  $\frac{1}{2} < \alpha \leq 1$ . This indicates that, for  $k=1,2,\ldots,k_0$ , the k Ritz values  $\theta_i^{(k)}$  may not approximate the first k large singular values  $\sigma_i$  in natural order and particularly there is at least one Ritz value  $\theta_{k_0}^{(k_0)} < \sigma_{k_0+1}$ , causing that  $x^{(k_0)}$  is already deteriorated and cannot be as accurate as the best TSVD solution  $x_{k_0}^{tsvd}$ , so that LSQR has only the partial regularization. We can also make use of Theorem 4 to explain the partial regularization of LSQR: Theorem 3 has shown that  $\|\Delta_k\|$  is generally not small and may become arbitrarily large as k increases up to  $k_0$  for mildly ill-posed problems, meaning that  $\|\sin\Theta(\mathcal{V}_k,\mathcal{V}_k^R)\| \approx 1$ , as the sharp bound (52) indicates, from which it follows that a small Ritz value  $\theta_{k_0}^{(k_0)} < \sigma_{k_0+1}$  generally appears.

### 5 Decay rates of $\alpha_k$ and $\beta_{k+1}$ and their practical importance

In this section, we will present a number of results on the decay rates of  $\alpha_k$  and  $\beta_{k+1}$ . The decay rates of  $\alpha_k$  and  $\beta_{k+1}$  are particularly useful for practically detecting the degree of ill-posedness of (1) and identifying the full or partial regularization of LSQR. We prove how  $\alpha_k$  and  $\beta_{k+1}$  decay by relating them to  $\gamma_k$  and the estimates established for it. Then we show how to exploit the decay rate of  $\alpha_k + \beta_{k+1}$  to identify the degree of ill-posedness of (1) and the regularization of LSQR.

**Theorem 9** With the notation defined previously, the following results hold:

$$\alpha_{k+1} < \gamma_k \le \sqrt{1 + \eta_k^2} \sigma_{k+1}, \ k = 1, 2, \dots, n-1,$$
 (111)

$$\beta_{k+2} < \gamma_k \le \sqrt{1 + \eta_k^2} \sigma_{k+1}, \ k = 1, 2, \dots, n-1,$$
 (112)

$$\alpha_{k+1}\beta_{k+2} \le \frac{\gamma_k^2}{2} \le \frac{(1+\eta_k^2)\sigma_{k+1}^2}{2}, \ k=1,2,\ldots,n-1,$$
 (113)

$$\gamma_{k+1} < \gamma_k, \ k = 1, 2, \dots, n-2.$$
 (114)

*Proof.* From (108), since P and  $Q_n$  are orthogonal matrices, we have

$$\gamma_k = \|A - P_{k+1} B_k Q_k^T\| = \|P^T (A - P_{k+1} B_k Q_k^T) Q_n\|$$
(115)

$$= \left\| \begin{pmatrix} B_n \\ \mathbf{0} \end{pmatrix} - (I, \mathbf{0})^T B_k(I, \mathbf{0}) \right\| = \|G_k\|$$
 (116)

with

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

$$(117)$$

resulting from deleting the  $(k+1) \times k$  leading principal matrix of  $B_n$  and the first k zero rows and columns of the resulting matrix. From the above, for k = 1, 2, ..., n-1 we have

$$\alpha_{k+1}^2 + \beta_{k+2}^2 = \|G_k e_1\|^2 \le \|G_k\|^2 = \gamma_k^2, \tag{118}$$

which shows that  $\alpha_{k+1} < \gamma_k$  and  $\beta_{k+2} < \gamma_k$  since  $\alpha_{k+1} > 0$  and  $\beta_{k+2} > 0$ . So from (83), we get (111) and (112). On the other hand, noting that

$$2\alpha_{k+1}\beta_{k+2} \le \alpha_{k+1}^2 + \beta_{k+2}^2 \le \gamma_k^2$$

we get (113).

Note that  $\alpha_k > 0$  and  $\beta_{k+1} > 0$ , k = 1, 2, ..., n. By  $\gamma_k = ||G_k||$  and (117), note that  $\gamma_{k+1} = ||G_{k+1}||$  equals the 2-norm of the submatrix deleting the first column of  $G_k$ . Applying the Cauchy's strict interlacing theorem to the singular values of this submatrix and  $G_k$ , we obtain (114).

Remark 20 For severely and moderately ill-posed problems, based on the results in the last section, (111) and (112) show that  $\alpha_{k+1}$  and  $\beta_{k+2}$  decay as fast as  $\sigma_{k+1}$  for  $k \le k_0$  and their decays may become slow for  $k > k_0$ . For mildly ill-posed problems, since  $\eta_k$  are generally bigger than one considerably for  $k \le k_0$ ,  $\alpha_{k+1}$  and  $\beta_{k+2}$  cannot generally decay as fast as  $\sigma_{k+1}$ , and their decays become slower for  $k > k_0$ .

We now shed light on (111) and (112). For a given (1), its degree of ill-posedness is either known or unknown. If it is unknown, (111) is of practical importance and can be exploited to identify whether or not LSQR has the full regularization without extra cost in an automatic and reliable way, so is (112). From the proofs of (111) and (112), we find that  $\alpha_{k+1}$  and  $\beta_{k+2}$  are as small as  $\gamma_k$ . Since our theory and analysis in Section 4 have proved that  $\gamma_k$  decays as fast as  $\sigma_{k+1}$  for severely or moderately ill-posed problems with  $\rho > 1$  or  $\alpha > 1$  suitably and it decays more slowly than  $\sigma_{k+1}$  for mildly il-posed problems, the decay rate of  $\sigma_k$  can be judged by that of  $\alpha_k$  or  $\beta_{k+1}$  or better judged by that of  $\alpha_k + \beta_{k+1}$  reliably, as shown below.

Given (1), run LSQR until semi-convergence occurs at iteration  $k^*$ . Check how  $\alpha_k + \beta_{k+1}$  decays as k increases during the process. If, on average, it decays in an obviously exponential way, then (1) is a severely ill-posed problem. In this case, LSQR has the full regularization, and semi-convergence means that we have found a best possible regularized solution. If, on average,  $\alpha_k$  decays as fast as  $k^{-\alpha}$  with  $\alpha > 1$  considerably, then (1) is surely a moderately ill-posed problem, and LSQR also has found a best possible regularized solution at semi-convergence. If, on average, it decays at most as fast as or more slowly than  $k^{-\alpha}$  with  $\alpha$  no more than one, (1) is a mildly ill-posed problem. Notice that the noise e does not deteriorate regularized solutions until semi-convergence. Therefore, if a hybrid LSQR is used, then it is more reasonable and also cheaper to apply regularization to projected problems only from iteration  $k^* + 1$  onwards other than from the first iteration, as done in the hybrid Lanczos bidiagonalization/Tikhonov regularization scheme [8], until a best possible regularized solution is found.

## 6 Numerical experiments

Huang and Jia [56] have numerically justified the full regularization of LSQR for severely and moderately ill-posed problems and its partial regularization for mildly ill-posed problems [45], where each A is  $1,024 \times 1,024$ . In this section, we report numerical experiments to confirm our theory and illustrate the full or partial regularization of LSQR in much more detail. For the first two kinds of problems, we demonstrate that  $\gamma_k$ ,  $\alpha_{k+1}$  and  $\beta_{k+2}$  decay as fast as  $\sigma_{k+1}$ . We compare LSQR and the hybrid LSQR with the TSVD method applied to projected problems after semi-convergence. For each of severely and moderately ill-posed problems, we show that the regularized solution obtained by LSQR at semi-convergence is at least as accurate as the best TSVD regularized solution, indicating that LSQR has the full regularization. In the meantime, for mildly ill-posed problems, we show that the regularized solution obtained by LSQR at semi-convergence is considerably less accurate than  $x_{k0}^{ISVd}$ , demonstrating that LSQR has only the partial regularization.

We choose several ill-posed problems from Hansen's regularization toolbox [45], which include the severely ill-posed problems shaw, wing, the moderately ill-posed problems heat, phillips, and the mildly ill-posed problem deriv2 with the parameter "example=3". All the codes are from [45], and the problems arise from discretizations of (2). We remind that, as far as solving (1) is concerned, our primary goal consists in justifying the regularizing effects of iterative solvers for (1), which are unaffected by the size of (1) and only depends on the degree of ill-posedness, the noise level ||e||and the actual discrete Picard condition, provided that the condition number of (1), measured by the ratio between the largest and smallest singular values of each A, is large enough. Therefore, for this purpose, as extensively done in the literature (see, e.g., [44,47] and the references therein as well as many other papers), it is enough to report the results on small and/or medium sized discrete ill-posed problems since the condition numbers of these A are already huge or large, which, in finite precision arithmetic, are roughly  $10^{16}$ ,  $10^8$  and  $10^6$  for severely, moderately and mildly illposed problems with n = 256, respectively. Indeed, for n large, say, 10,000 or more, we have observed that LSQR has the same behavior as for small n, e.g., n = 256, which is used in this paper. The only exception is deriv2, and we will test a larger one of n = 3,000 whose condition number is one order larger than that of n = 256, so as to better confirm the partial regularization of LSQR. Also, an important reason is that such choice enables us to fully justify the regularization effects of LSQR by comparing it with the TSVD method, which suits only for small and/or medium sized problems because of its computational complexity. For each example, we generate A,  $x_{true}$  and  $\hat{b}$ . In order to simulate the noisy data, we generate white noise vectors e such that the relative noise levels  $\varepsilon = \frac{\|e\|}{\|\hat{b}\|} = 10^{-2}, 10^{-3}, 10^{-4}$ , respectively. To simulate exact arithmetic, LSQR uses full reorthogonalization in Lanczos bidiagonalization. All the computations are carried out in Matlab 7.8 with the machine precision  $\varepsilon_{\text{mach}}$  =  $2.22 \times 10^{-16}$  under the Miscrosoft Windows 7 64-bit system.

### 6.1 The accuracy of rank k approximations

In Figure 1, we display the decay curves of the  $\gamma_k$  for shaw with  $\varepsilon = 10^{-2}, 10^{-3}$  and for wing with  $\varepsilon = 10^{-3}, 10^{-4}$ , respectively. We observe that the three curves with different  $\varepsilon$  are almost unchanged. This is in accordance with our Remark 11, where it is stated that the decay rate of  $\gamma_k$  is little affected by noise levels for severely ill-posed problems, since  $\gamma_k$  primarily depends on the decay rate of  $\sigma_{k+1}$  and different noise levels only affect the value of  $\kappa_0$  other than the decay rate of  $\kappa_0$ . In addition, we have observed that  $\kappa_0$  and  $\kappa_0$  until they level off at  $\kappa_0$  due to round-off errors. Most importantly, the results have clearly confirmed the theory that  $\kappa_0$  decreases as fast as  $\kappa_0$ , and we have  $\kappa_0$  and  $\kappa_0$ , whose decay curves are almost indistinguishable.

In Figure 2, we plot the relative errors  $||x^{(k)} - x_{true}|| / ||x_{true}||$  with different  $\varepsilon$  for these two problems. As we have seen, LSQR exhibits clear semi-convergence. Moreover, for a smaller  $\varepsilon$ , we get a more accurate regularized solution at cost of more iterations, as  $k_0$  is bigger from (7) and (8).

From Figure 3, we see that  $\gamma_k$  decreases almost as fast as  $\sigma_{k+1}$  for the moderately ill-posed problems heat and phillips. However, slightly different from severely ill-

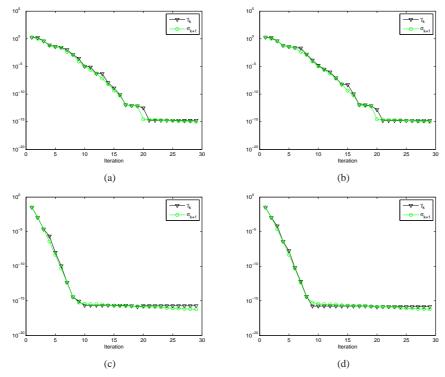


Fig. 1 (a)-(b): Decay curves of the sequences  $\gamma_k$  and  $\sigma_{k+1}$  for shaw with  $\varepsilon=10^{-2}$  (left) and  $\varepsilon=10^{-3}$  (right); (c)-(d): Decay curves of the sequences  $\gamma_k$  and  $\sigma_{k+1}$  for wing with  $\varepsilon=10^{-3}$  (left) and  $\varepsilon=10^{-4}$  (right).

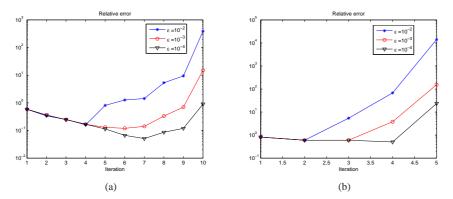


Fig. 2 The relative errors  $||x^{(k)} - x_{true}|| / ||x_{true}||$  with  $\varepsilon = 10^{-2}, 10^{-3}, 10^{-4}$  for shaw (left) and wing (right).

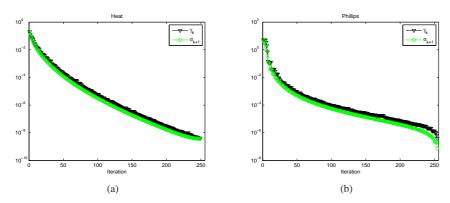


Fig. 3 (a): Decay curves of the sequences  $\gamma_k$  and  $\sigma_{k+1}$  for heat with (left) and (b): Decay curves of the sequences  $\gamma_k$  and  $\sigma_{k+1}$  for phillips with  $\varepsilon = 10^{-3}$  (right).

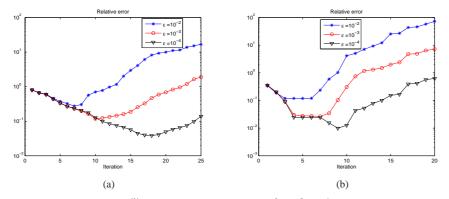


Fig. 4 The relative errors  $||x^{(k)} - x_{true}|| / ||x_{true}||$  with  $\varepsilon = 10^{-2}, 10^{-3}, 10^{-4}$  for heat (left) and phillips (right).

posed problems,  $\gamma_k$ , though excellent approximations to  $\sigma_{k+1}$ , may not be so very accurate. This is expected, as the constants  $\eta_k$  in (85) are generally bigger than those in (84) for severely ill-posed problems. Also, different from Figure 1, we observe from Figure 3 that  $\gamma_k$  deviates more from  $\sigma_{k+1}$  with k increasing, especially for the problem phillips. This confirms Remarks 11–13 on moderately ill-posed problems.

In Figure 4, we depict the relative errors of  $x^{(k)}$ , and from them we observe analogous phenomena to those for severely ill-posed problems. The only distinction is that LSQR now needs more iterations, i.e., a bigger  $k_0$  is needed for moderately ill-posed problems with the same  $\varepsilon$ , as is seen from (7) and (8).

Figure 5 (a)-(b) display the decay curves of the partial and complete sequences  $\gamma_k$  and  $\sigma_{k+1}$  for the mildly ill-posed problem deriv2, respectively. We see that, different from severely and moderately ill-posed problems,  $\gamma_k$  does not decay so fast as  $\sigma_{k+1}$  and deviates from  $\sigma_{k+1}$  significantly. These observations justify our theory and confirm that the rank k approximations to k generated by Lanczos bidiagonalization are not as accurate as those for severely and moderately problems.

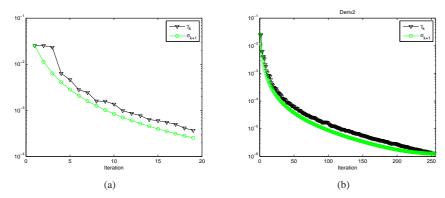


Fig. 5 (a)-(b): Decay curves of the partial and complete sequences  $\gamma_k$  and  $\sigma_{k+1}$  for deriv2 with  $\varepsilon = 10^{-3}$ 

#### 6.2 Decay behavior of $\alpha_k$ and $\beta_{k+1}$

For the severely ill-posed shaw, wing and the moderately ill-posed heat, phillips, we now illustrate that  $\alpha_k$  and  $\beta_{k+1}$  decay as fast as the singular values  $\sigma_k$  of A. We take the noise level  $\varepsilon = 10^{-3}$ . The results are similar for  $\varepsilon = 10^{-2}$  and  $10^{-4}$ .

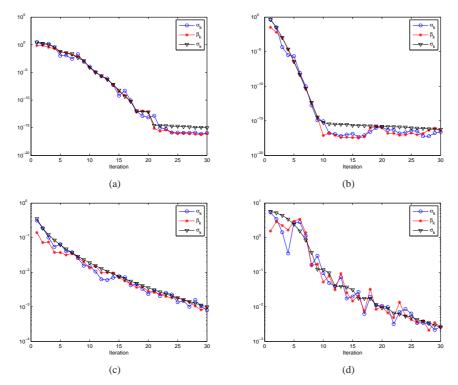
Figure 6 illustrates that both  $\alpha_k$  and  $\beta_{k+1}$  decay as fast as  $\sigma_k$ , and for shaw and wing all of them decay swiftly and level off at  $\varepsilon_{\text{mach}}$  due to round-off errors in finite precision arithmetic. Precisely, they reach the level of  $\varepsilon_{\text{mach}}$  at k=22 and k=8 for shaw and wing, respectively. Such decay behavior has also been observed in [7,26, 29], but no theoretical support was given. These experiments confirm Theorem 6 and Theorem 9, which have proved that  $\gamma_k$  decreases as fast as  $\sigma_{k+1}$  and that  $\alpha_k$ ,  $\beta_{k+1}$  and  $\alpha_k + \beta_{k+1}$  decay as fast as  $\sigma_k$ .

#### 6.3 A comparison of LSQR and the TSVD method

We compare the performance of LSQR and the TSVD method for the severely ill-posed shaw, wing, the moderately ill-posed heat, phillips and the mildly ill-posed problem deriv2 of n=3,000. We take  $\varepsilon=10^{-3}$ . For each problem, we compute the relative errors of regularized solutions and the residual norms obtained by the two methods. We will demonstrate that LSQR has the full regularization for the severely and moderately ill-posed problems, but it has only the partial regularization for the mildly ill-posed problem. The results on  $\varepsilon=10^{-2},\ 10^{-4}$  are very similar, and we thus omit them.

Figures 7–8 indicate LSQR and the TSVD method behave very similarly for shaw and wing. They illustrate that, for wing, the norms of approximate solutions and the relative errors by the two methods are almost indistinguishable for the same k, and, for shaw, the residual norms by LSQR decreases more quickly than the ones by the TSVD method for k = 1, 2, 3 and then they become almost identical starting from k = 4. These results demonstrate that LSQR has the full regularization.

For each of heat and phillips, Figures 9–10 demonstrate that the best regularized solution obtained by LSQR is at least as accurate as, in fact, a little bit more accurate



**Fig. 6** (a)-(d): Decay curves of the sequences  $\alpha_k$ ,  $\beta_{k+1}$  and  $\sigma_k$  for shaw, wing, i\_laplace and heat (from top left to bottom right).

than that by the TSVD method, and the corresponding residual norms decreases and drop below at least the same level as those by the TSVD method. The residual norms by the two methods then stagnate after the best regularized solutions are found. All these confirm that LSQR has the full regularization.

To better illustrate the regularizing effects of LSQR, we test a larger deriv2 of n=3000 whose condition number is  $1.1\times10^7$ . Figure 11 demonstrates that the best regularized solution by LSQR at semi-convergence is considerably less accurate than  $x_{k_0}^{tsvd}$ . Actually, the relative error of the former is  $8.0\times10^{-3}$ , while that of the latter is only  $1.1\times10^{-3}$ , almost one order more accurate. As we have observed, the semi-convergence of LSQR occurs at the very first iteration, while the best regularized solution  $x_{k_0}^{tsvd}$  consists of three dominant SVD components of A. The results clearly shows that LSQR has only the partial regularization for mildly ill-posed problems.

From the figures we observe some obvious differences between moderately and severely ill-posed problems. For heat, it is seen that the relative errors and residual norms converge considerably more quickly for the LSQR solutions than for the TSVD solutions. Figure 9 (a) tells us that LSQR only uses 12 iterations to find the best regularized solution, but the TSVD method finds the best regularized solution for

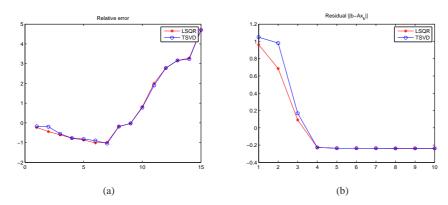


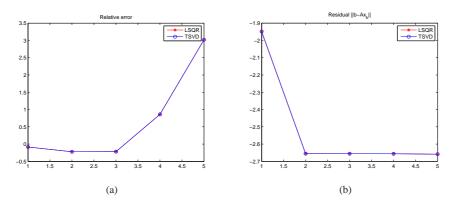
Fig. 7 Results for the severely ill-posed problem shaw.

 $k_0 = 21$ . Similar differences are observed for phillips, where Figure 10 (a) indicates that both LSQR and the TSVD method find the best regularized solutions at  $k_0 = 7$ .

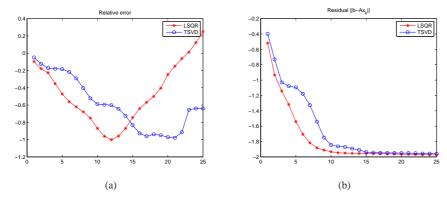
We can observe more. Figure 9 shows that the TSVD solutions improve little and their residual norms decrease very slowly for the indices i = 4,5,11,12,18,19,20. This implies that the  $v_i$  corresponding to these indices i make very little contribution to the TSVD solutions. This is due to the fact that the Fourier coefficients  $|u_i^T \hat{b}|$ are very small relative to  $\sigma_i$  for these indices i. Note that  $\mathcal{K}_k(A^TA, A^Tb)$  adapts itself in an optimal way to the specific right-hand side b, while the TSVD method uses all  $v_1, v_2, \dots, v_k$  to construct a regularized solution, independent of b. Therefore,  $\mathcal{K}_k(A^TA, A^Tb)$  picks up only those SVD components making major contributions to  $x_{true}$ , such that LSQR uses possibly fewer k iterations than  $k_0$  needed by the TSVD method to capture those truly needed dominant SVD components. The fact that LSOR (CGLS) includes fewer SVD components than the TSVD solution with almost the same accuracy was first noticed by Hanke [38]. Generally, for severely and moderately ill-posed problems, we may deduce that LSQR uses possibly fewer than  $k_0$  iterations to compute a best possible regularized solution if, in practice, some of  $|u_i^T b|$ ,  $i = 1, 2, ..., k_0$  are considerably bigger than the corresponding  $\sigma_i$  and some of them are reverse. For phillips, as noted by Hansen [47, p.32, 123-125], half of the SVD components satisfy  $u_i^T \hat{b} = v_i^T x_{true} = 0$  for i even, only the odd indexed  $v_1, v_3, \ldots$ , make contributions to  $x_{true}$ . This is why the relative errors and residual norms of TSVD solutions do not decrease at even indices before  $x_{k_0}^{tsvd}$  is found.

# 7 Conclusions

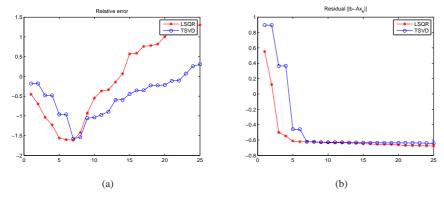
For the large-scale (1), iterative solvers are the only viable approaches. Of them, LSQR and CGLS are most popularly used for general purposes, and CGME and LSMR are also choices. They have general regularizing effects and exhibit semi-convergence. However, if semi-convergence occurs before it captures all the needed dominant SVD components, then best possible regularized solutions are not yet found and the solvers have only the partial regularization. In this case, their hybrid variants have often been used to compute best possible regularized solutions. If semi-



 $\textbf{Fig. 8} \ \ \text{Results for the severely ill-posed problem wing.}$ 



 $\label{Fig.9} Fig.\,9\ \mbox{Results for the moderately ill-posed problem heat}.$ 



 $\textbf{Fig. 10} \ \ \text{Results for the moderately ill-posed problem phillips}.$ 

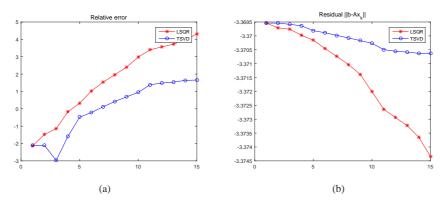


Fig. 11 Results for the moderately ill-posed problem phillips.

convergence means that they have already found best possible regularized solutions, they have the full regularization, and we simply stop them after semi-convergence.

For the case that the singular values of A are all simple, we have considered the fundamental open question in depth: Do LSQR and CGLS have the full or partial regularization for severely, moderately and mildly ill-posed problems? We have first considered the case that all the singular values of A are simple. As a key and indispensable step, we have established accurate bounds for the 2-norm distances between the underlying k dimensional Krylov subspace and the k dimensional dominant right singular subspace for the three kinds of ill-posed problems under consideration. Then we have provided other absolutely necessary background and ingredients. Based on them, we have proved that, for severely or moderately ill-posed problems with  $\rho > 1$ or  $\alpha > 1$  suitably, LSQR has the full regularization. Precisely, for  $k \le k_0$  we have proved that a k-step Lanczos bidiagonalization produces a near best rank k approximation of A and the k Ritz values approximate the first k large singular values of A in natural order, and no small Ritz value smaller than  $\sigma_{k_0+1}$  appears before a best possible regularized solution has been found. For mildly ill-posed problems, we have proved that LSQR generally has only the partial regularization since a small Ritz value generally appears before all the needed dominant SVD components are captured. Since CGLS is mathematically equivalent to LSQR, our assertions on the full or partial regularization of LSQR apply to CGLS as well.

We have derived bounds for the diagonals and subdiagonals of bidiagonal matrices generated by Lanczos bidiagonalization. Particularly, we have proved that they decay as fast as the singular values of A for severely ill-posed problems or moderately ill-posed problems with  $\rho>1$  or  $\alpha>1$  suitably and decay more slowly than the singular values of A for mildly ill-posed problems. These bounds are of theoretical and practical importance, and they can be used to identify the degree of ill-posedness without extra cost and decide the full or partial regularization of LSQR. We have made detailed and illuminating numerical experiments, confirming our theory.

Our analysis approach can be adapted to MR-II for symmetric ill-posed problems, and certain definitive assertions are expected for three kinds of symmetric ill-posed problems. Our approach are applicable to the preconditioned CGLS (PCGLS) and

LSQR (PLSQR) [44,47] by exploiting the transformation technique originally proposed in [12] and advocated in [35,39,45] or the preconditioned MR-II [47,48], all of which correspond to a general-form Tikhonov regularization involving the matrix pair  $\{A,L\}$ , in which the regularization term  $\|x\|^2$  is replaced by  $\|Lx\|^2$  with some  $p \times n$  matrix  $L \neq I$ . It should also be applicable to the mathematically equivalent LSQR variant [65] that is based on a joint bidiagonalization of the matrix pair  $\{A,L\}$  that corresponds to the above general-form Tikhonov regularization. In this setting, the Generalized SVD (GSVD) of  $\{A,L\}$  or the mathematically equivalent SVD of  $AL_A^\dagger$  will replace the SVD of A to play a central role in analysis, where  $L_A^\dagger = \left(I - \left(A(I-L^\dagger L)^\dagger A\right)\right)^\dagger L^\dagger$  is call the A-weighted generalized inverse of L and  $L_A^\dagger = L^{-1}$  if L is square and invertible; see [44, p.38-40,137-38] and [47, p.177-183].

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