

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

ZHONGXIAO JIA<sup>†</sup>

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

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

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

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

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

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

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

where the kernel  $k(s, t) \in L^2(\Omega \times \Omega)$  and  $g(s)$  are known functions, while  $x(t)$  is the unknown function to be sought. If  $k(s, t)$  is non-degenerate and  $g(s)$  satisfies the Picard condition, there exists the unique square integrable solution  $x(t)$ ; see [17, 36, 39, 56, 62]. 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, ground-water modeling, and many others; see, e.g., [1, 16, 17, 39, 47, 52, 53, 56, 62, 63, 90]. The theory and numerical treatments of (1.2) can be found in [56, 57]. The right-hand side  $b = b_{true} + e$  is noisy and assumed to be contaminated by a Gaussian white noise

\*This work was supported in part by the National Science Foundation of China (No. 11771249).

<sup>†</sup>Department of Mathematical Sciences, Tsinghua University, 100084 Beijing, China. (jiazx@tsinghua.edu.cn)

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

We assume that  $b_{true}$  satisfies the discrete Picard condition  $\|A^\dagger b_{true}\| \leq C$  with some constant  $C$  for  $\|A^\dagger\|$  arbitrarily large [1, 22, 33, 34, 36, 39, 53]. It is a discrete analog of the Picard condition in the Hilbert space setting; see, e.g., [33], [36, p.9], [39, p.12] and [53, p.63]. Without loss of generality, assume that  $Ax_{true} = b_{true}$ . Then for a Gaussian white noise  $e$ , the two dominating regularization approaches are to solve the following two equivalent problems:

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

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

$$(1.4) \quad \min_{x \in \mathbb{R}^n} \{\|Ax - b\|^2 + \lambda^2 \|Lx\|^2\}$$

with  $\lambda > 0$  the regularization parameter [36, 39, 73, 82, 83], where  $L$  is a regularization matrix, and its suitable choice is based on a-prior information on  $x_{true}$ . Typically,  $L$  is either the identity matrix  $I$  or the scaled discrete approximation of a first or second order derivative operator. If  $L = I$ , the identity matrix, (1.3) reduces to standard-form regularization in 2-norm, and (1.4) is standard-form Tikhonov regularization, both of which are *2-norm filtering* regularization problems.

We are concerned with the case  $L = I$  in this paper. If  $L \neq I$ , (1.3) and (1.4), in principle, can be transformed into standard-form problems [36, 39]. In this case, the solutions of (1.1), (1.3) and (1.4) can be fully analyzed by the singular value decomposition (SVD) of  $A$ . Let

$$(1.5) \quad A = U \begin{pmatrix} \Sigma \\ \mathbf{0} \end{pmatrix} V^T$$

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

$$(1.6) \quad x_{naive} = \sum_{i=1}^n \frac{u_i^T b}{\sigma_i} v_i = \sum_{i=1}^n \frac{u_i^T b_{true}}{\sigma_i} v_i + \sum_{i=1}^n \frac{u_i^T e}{\sigma_i} v_i = x_{true} + \sum_{i=1}^n \frac{u_i^T e}{\sigma_i} v_i$$

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

The discrete Picard condition means that, on average, the Fourier coefficient  $|u_i^T b_{true}|$  decays faster than  $\sigma_i$  and enables regularization to compute useful approximations to  $x_{true}$ . The following popular simplifying model is used throughout Hansen's books [36, 39] and the references therein as well as the current paper:

$$(1.7) \quad |u_i^T b_{true}| = \sigma_i^{1+\beta}, \quad \beta > 0, \quad i = 1, 2, \dots, n,$$

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

The Gaussian white noise  $e$  has a number of attractive properties which play a critical role in the regularization analysis: Its covariance matrix is  $\eta^2 I$ , the expected values  $\mathcal{E}(\|e\|^2) = m\eta^2$  and  $\mathcal{E}(|u_i^T e|) = \eta$ ,  $i = 1, 2, \dots, n$ , so that  $\|e\| \approx \sqrt{m}\eta$  and  $|u_i^T e| \approx \eta$ ,  $i = 1, 2, \dots, n$ ; see, e.g., [36, p.70-1] and [39, p.41-2]. The noise  $e$  thus affects  $u_i^T b$ ,  $i = 1, 2, \dots, n$ , *more or less equally*. With (1.7), relation (1.6) shows that for large singular values the signal terms  $|u_i^T b_{true}|/\sigma_i$  are dominant relative to the noise terms  $|u_i^T e|/\sigma_i$ , that is, the  $\sigma_i^\beta$  are considerably bigger than the  $\eta/\sigma_i$ . Once  $|u_i^T b_{true}| \leq |u_i^T e|$  for small singular values, the noise  $e$  dominates  $|u_i^T b|$ , and the terms  $\frac{|u_i^T b|}{\sigma_i} \approx \frac{|u_i^T e|}{\sigma_i}$  overwhelm  $x_{true}$  and thus must be filtered out. The transition or cutting-off point  $k_0$  is such that

$$(1.8) \quad |u_{k_0}^T b| \approx |u_{k_0}^T b_{true}| > |u_{k_0}^T e| \approx \eta, \quad |u_{k_0+1}^T b| \approx |u_{k_0+1}^T e| \approx \eta;$$

see [39, p.42, 98] and a similar description [36, p.70-1]. In this sense, the  $\sigma_k$  are divided into the  $k_0$  large ones and the  $n - k_0$  small ones.

The truncated SVD (TSVD) method [33, 36, 39] is a reliable and effective method for solving small to medium sized (1.3), and it deals with a sequence of problems

$$(1.9) \quad \min \|x\| \quad \text{subject to} \quad \|A_k x - b\| = \min$$

starting with  $k = 1$  onwards, where  $A_k = U_k \Sigma_k V_k^T$  is the best rank  $k$  approximation to  $A$  with respect to the 2-norm with  $U_k = (u_1, \dots, u_k)$ ,  $V_k = (v_1, \dots, v_k)$  and  $\Sigma_k = \text{diag}(\sigma_1, \dots, \sigma_k)$ ; it holds that  $\|A - A_k\| = \sigma_{k+1}$  [8, p.12]. The solution to (1.9) is  $x_k^{tsvd} = A_k^\dagger b$ , called the TSVD regularized solution, which is the minimum 2-norm solution to  $\min_{x \in \mathbb{R}^n} \|A_k x - b\|$  that replaces  $A$  by  $A_k$  in (1.1).

Based on the above properties of the Gaussian white noise  $e$ , it is known from [36, p.70-1] and [39, p.71,86-8,95] that the TSVD solutions

$$(1.10) \quad x_k^{tsvd} = A_k^\dagger b = \begin{cases} \sum_{i=1}^k \frac{u_i^T b}{\sigma_i} v_i \approx \sum_{i=1}^k \frac{u_i^T b_{true}}{\sigma_i} v_i, & k \leq k_0; \\ \sum_{i=1}^k \frac{u_i^T b}{\sigma_i} v_i \approx \sum_{i=1}^{k_0} \frac{u_i^T b_{true}}{\sigma_i} v_i + \sum_{i=k_0+1}^k \frac{u_i^T e}{\sigma_i} v_i, & k > k_0, \end{cases}$$

and  $x_{k_0}^{tsvd}$  is the best TSVD regularized solution of (1.1); we have  $\|x_{true} - x_{k_0}^{tsvd}\| = \min_{k=1,2,\dots,n} \|x_{true} - x_k^{tsvd}\|$ , which balances the regularization error  $(A^\dagger - A_k^\dagger) b_{true}$  and the perturbation error  $A_k^\dagger e$  optimally, and  $\|A x_k^{tsvd} - b\| \approx \|e\|$  stabilizes for  $k$  not close to  $n$  after  $k > k_0$ . The index  $k$  plays the role of the regularization parameter.

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

$$(1.11) \quad x_\lambda = \sum_{i=1}^n f_i \frac{u_i^T b}{\sigma_i} v_i,$$

where the  $f_i = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2}$  are filters. The error  $x_\lambda - x_{true}$  can be written as the sum of the regularization error  $((A^T A + \lambda^2 I)^{-1} A^T - A^\dagger) b_{true}$  and the perturbation error  $(A^T A + \lambda^2 I)^{-1} A^T e$ , and an optimal  $\lambda_{opt}$  is such that  $\|x_{true} - x_{\lambda_{opt}}\| = \min_{\lambda \geq 0} \|x_{true} - x_\lambda\|$  and balances these two errors [36, 39, 56, 90]. In the spirit of  $x_{k_0}^{tsvd}$ , the best Tikhonov 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 [36, 39], that is,  $\lambda_{opt}$  must be such that  $f_i = \mathcal{O}(1)$ ,  $i = 1, 2, \dots, k_0$  and  $f_i/\sigma_i \approx 0$ ,  $i = k_0 + 1, \dots, n$ . Therefore, it is expected that  $x_{k_0}^{tsvd}$  and  $x_{\lambda_{opt}}$  have very similar accuracy. Indeed, it has been observed and justified that these two regularized solutions essentially have the minimum 2-norm error; see [34], [36, p.109-11], [39, Sections 4.2 and 4.4] and [88].

As a matter of fact, there is solid mathematical theory on the TSVD method and standard-form Tikhonov regularization: for an underlying linear compact equation  $Kx = g$ , e.g., (1.2), with the noisy  $g$  and true solution  $x_{true}$ , under the source condition that its solution  $x_{true} \in \mathcal{R}(K^*)$  or  $x_{true} \in \mathcal{R}(K^*K)$ , the range of the adjoint  $K^*$  of  $K$  or that of  $K^*K$ , the errors of  $x_{k_0}^{tsvd}$  and  $x_{\lambda_{opt}}$  are *order optimal*, i.e., *the same order as the worst-case error* [56, p.13,18,20,32-40], [63, p.90] and [90, p.7-12]. These conclusions carries over to (1.1) [90, p.8]. Therefore, when only deterministic 2-norm filtering methods are taken into account, both  $x_{\lambda_{opt}}$  and  $x_{k_0}^{tsvd}$  are best possible solutions to (1.1) under the above assumptions. More generally, for  $x_{true} \in \mathcal{R}((K^*K)^{\beta/2})$  with any  $\beta > 0$ , the error of the TSVD solution  $x_{k_0}^{tsvd}$  is always order optimal, while  $x_{\lambda_{opt}}$  is best possible only for  $\beta \leq 2$ ; see [17, Chap. 4-5] for details.

As a consequence, we can take  $x_{k_0}^{tsvd}$  as the reference standard when assessing the accuracy of the 2-norm filtering best regularized solution obtained by a regularization method. In other words, we take the TSVD method as reference standard to evaluate the regularization ability of a deterministic 2-norm filtering regularization method.

A number of parameter-choice methods have been developed for finding  $\lambda_{opt}$  or  $k_0$ , such as the discrepancy principle [61], the L-curve criterion, whose use goes back to Miller [60] and Lawson and Hanson [58] and is termed much later and studied in detail in [35, 40], the generalized cross validation (GCV) [27, 91], and the method based on error estimation [24, 74]; see, e.g., [3, 17, 36, 39, 53, 54, 55, 65, 90] for numerous comparisons. Each of these methods has its own merits and disadvantages, and none is absolutely reliable for all discrete ill-posed problems. For example, some of them may fail to find accurate approximations to  $\lambda_{opt}$ ; see [30, 89] for an analysis on the L-curve criterion method and [36] for some other parameter-choice methods.

For  $A$  large, the TSVD method and the Tikhonov regularization method are generally too demanding, and only iterative regularization methods are computationally viable. Krylov solvers are a major class of iterative methods for solving a large scale (1.1), and they project (1.1) onto a sequence of low dimensional Krylov subspaces and computes iterates to approximate  $x_{true}$  [1, 17, 26, 29, 36, 39, 56]. Of them, the CGLS (or CGNR) method, which implicitly applies the CG method [28, 42] to  $A^T Ax = A^T b$ , and its mathematically equivalent LSQR algorithm [70] have been most commonly used. The Krylov solvers CGME (or CGNE) [8, 9, 14, 29, 31] and LSMR [9, 19] have been also choices, which amount to the CG method applied to  $\min \|AA^T y - b\|$  or  $AA^T y = b$  with  $x = A^T y$  and MINRES [69] applied to  $A^T Ax = A^T b$ , respectively. These Krylov solvers have been intensively studied and known to have general regularizing effects [1, 15, 26, 29, 31, 36, 39, 43, 44] and exhibit semi-convergence [63, p.89]; see also [8, p.314], [9, p.733], [36, p.135] and [39, p.110]: the iterates converge to  $x_{true}$  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  $x_{naive}$ . 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 not only due to the increasingly ill-conditioning of the projected problem, but also to the fact that the noise progressively enters the approximation subspace [44].

The behavior of ill-posed problems critically depends on the decay rate of  $\sigma_j$ .

The following characterization of the degree of ill-posedness of (1.1) was introduced in [45] and has been widely used [1, 17, 36, 39, 62]: if  $\sigma_j = \mathcal{O}(\rho^{-j})$  with  $\rho > 1$ ,  $j = 1, 2, \dots, n$ , then (1.1) is severely ill-posed; if  $\sigma_j = \mathcal{O}(j^{-\alpha})$ , then (1.1) is mildly or moderately ill-posed for  $\frac{1}{2} < \alpha \leq 1$  or  $\alpha > 1$ . Here for mildly ill-posed problems we add the requirement  $\alpha > \frac{1}{2}$ , which does not appear in [45] but must be met for a linear compact operator equation [32, 36].

The regularizing effects of CG type methods were discovered in [51, 77, 81]. Johnson [51] had given a heuristic explanation on the success of CGLS. Based on these works, on page 13 of [10], Björck and Eldén in their 1979 survey foresightedly expressed a fundamental concern on CGLS (and LSQR): *More research is needed to tell for which problems this approach will work, and what stopping criterion to choose.* See also [36, p.145]. Hanke and Hansen [32] and Hansen [37] have addressed that a strict proof of the regularizing properties of conjugate gradients is extremely difficult.

An enormous effort has been made to the study of regularizing effects of LSQR and CGLS; see [18, 25, 29, 31, 36, 39, 43, 44, 46, 64, 67, 71, 76, 85], many of which concern the *asymptotic* behavior of the errors of  $x_{\lambda_{opt}}$  and  $x_{k_0}^{tsvd}$  as the noise  $e$ , which assumes no specific property, approaches zero in the Hilbert space setting. Our concern is to leave the *Gaussian white noise*  $e$  *fixed* and considers how the solution by LSQR and CGLS behaves as the regularization parameter varies in the *finite* dimensional space. Therefore, our analysis approach and results are *non-asymptotic* and different. It has long been well known [32, 36, 37, 39] and will also be elaborated in this paper that provided that the singular values of projected matrices in LSQR, called the Ritz values, always approximate the large singular values of  $A$  in natural order until semi-convergence, the best regularized solution obtained by LSQR is as accurate as  $x_{k_0}^{tsvd}$ . Such convergence is thus desirable. However, Hanke and Hansen [32], Hansen [36, 37, 39] and some others, e.g., Gazzola and Novati [22], address the difficulties to prove the convergence in this order. Hitherto there has been no general definitive and quantitative result on whether or not the Ritz values converge in this order for the three kinds of ill-posed problems.

Precisely, we now introduce such a definition: For the 2-norm filtering regularization problem (1.3), if a regularized solution is as accurate as  $x_{k_0}^{tsvd}$ , then it is called a 2-norm filtering best possible regularized solution. If a regularization method can compute such a best possible one, then it is said to have the *full* regularization in the sense of 2-norm filtering. Otherwise, it is said to have only the *partial* regularization.

In order to obtain a 2-norm filtering best possible solution of (1.1), LSQR and CGLS have been commonly combined with some explicit regularization [1, 6, 21, 36, 39]. CGLS is combined with the standard-form Tikhonov regularization, and it solves  $(A^T A + \lambda^2 I)x = A^T b$  for several regularization parameters  $\lambda$  and picks up a best solution [1, 20]. The hybrid LSQR variants have been advocated by Björck and Eldén [10] and O’Leary and Simmons [68], and improved and developed by Björck [7], Björck, Grimme and van Dooren [11], and Renaut, Vatankehah, and Ardestani [75]. They first project (1.1) onto Krylov subspaces and then regularize the projected problem explicitly at each iteration. They aim to remove the effects of small Ritz values and expands Krylov subspaces until they captures all the needed right singular vectors of  $A$ . The hybrid LSQR, CGME and LSMR have been intensively studied in, e.g., [4, 5, 6, 12, 13, 31, 32, 59, 66, 75] and [1, 39, 41]. For further information on hybrid methods, we refer to [23] and the references therein.

If an iterative solver is theoretically proved to have the full regularization, one can stop it after its semi-convergence is practically identified. To echo the concern of

Björck and Eldén, by the definition of the full or partial regularization, our question is: *Do LSQR, CGLS, LSMR and CGME have the full or partial regularization for severely, moderately and mildly ill-posed problems?* As we have seen, there has been no definitive answer to this long-standing fundamental question hitherto.

LSQR, CGME and LSMR are common in that, at iteration  $k$ , they are mathematically based on the same  $k$ -step Lanczos bidiagonalization process but compute *different* iterates from the *same*  $k$  dimensional right Krylov subspace. Remarkably, note that if the left and right subspaces are the dominant left and right singular subspaces  $\text{span}\{U_{k+1}\}$  (or  $\text{span}\{U_k\}$ ) and  $\text{span}\{V_k\}$  of  $A$  then the Ritz values of  $A$  with respect to them are exactly the first  $k$  large singular values of  $A$ . Therefore, whether or not the Ritz values converge to the large singular values of  $A$  in natural order critically depends on how the underlying  $k$  dimensional right Krylov subspace approaches  $\text{span}\{V_k\}$ . This paper concerns the fundamental problem that these methods face: How does the underlying  $k$  dimensional right Krylov subspace approximate  $\text{span}\{V_k\}$ ? Accurate solutions of this problem play a central role in analyzing the regularization ability of the mentioned four methods and in ultimately determining if each method has the full regularization. We will establish a general  $\sin \Theta$  theorem for the 2-norm distances between these two subspaces and derive accurate estimates on them for the three kinds of ill-posed problems. We notice that the  $\sin \Theta$  theorem involves some crucial quantities used to study the regularizing effects of LSQR [36, p.150-2], but there were no estimates for them there and in the literature.

In Section 2, we describe the Lanczos bidiagonalization process and the LSQR method, and make an introductory analysis. In Section 3 we make an analysis on the regularizing effects of LSQR and establish a basic result on its semi-convergence. In Section 4, we establish the  $\sin \Theta$  theorem for the 2-norm distance between the underlying  $k$  dimensional Krylov subspace and  $\text{span}\{V_k\}$ , and derive accurate estimates on them for the three kinds of ill-posed problems, which include accurate estimates for those key quantities in [36, p.150-2]. In Section 5 we consider the effects of the  $\sin \Theta$  theorem on the behavior of the smallest Ritz values involved in LSQR. We report a number of numerical examples to confirm our theory. Finally, we summarize the paper in Section 6.

Throughout the paper, we denote by  $\mathcal{K}_k(C, w) = \text{span}\{w, Cw, \dots, C^{k-1}w\}$  the  $k$  dimensional Krylov subspace generated by the matrix  $C$  and the vector  $w$ , and by  $I$  and the bold letter  $\mathbf{0}$  the identity matrix and the zero matrix with orders clear from the context, respectively. For the matrix  $B = (b_{ij})$ , we define  $|B| = (|b_{ij}|)$ , and for  $|C| = (|c_{ij}|)$ ,  $|B| \leq |C|$  means  $|b_{ij}| \leq |c_{ij}|$  componentwise.

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

**Algorithm 1:  $k$ -step Lanczos bidiagonalization process**

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

Algorithm 1 can be written in the matrix form

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

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

where  $e_{k+1}^{(k+1)}$  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

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

It is known from (2.1) that

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

The singular values  $\theta_i^{(k)}$ ,  $i = 1, 2, \dots, k$  of  $B_k$ , called the Ritz values of  $A$  with respect to the left and right subspaces  $\text{span}\{P_{k+1}\}$  and  $\text{span}\{Q_k\}$ , are all simple as  $\alpha_i > 0$ ,  $\beta_{i+1} > 0$ ,  $i = 1, 2, \dots, k$  provided that the algorithm does not break down.

Write  $\mathcal{V}_k^R = \mathcal{K}_k(A^T A, A^T b)$  and  $\mathcal{V}_k = \text{span}\{V_k\}$ . LSQR, CGME and LSMR LSQR, CGME and LSMR are based on the same Lanczos bidiagonalization process but extract *different* iterates from  $\mathcal{V}_k^R$ . We take LSQR as example. At iteration  $k$ , LSQR solves the problem

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

for the iterate

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

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

From  $\beta_1 e_1^{(k+1)} = P_{k+1}^T b$  and (2.5), we have

$$(2.6) \quad x_k^{lsqr} = Q_k B_k^\dagger P_{k+1}^T b,$$

that is,  $x_k^{lsqr}$  is the minimum 2-norm solution to the perturbed problem that replaces  $A$  in (1.1) by its rank  $k$  approximation  $P_{k+1} B_k Q_k^T$ . So LSQR solves a sequence of problems

$$(2.7) \quad \min \|x\| \quad \text{subject to} \quad \|P_{k+1} B_k Q_k^T x - b\| = \min$$

for the regularized solutions  $x_k^{lsqr}$  of (1.1) starting with  $k = 1$  onwards. Recall the TSVD method (cf. (1.9)) and that the best rank  $k$  approximation  $A_k$  to  $A$  satisfies  $\|A - A_k\| = \sigma_{k+1}$ . Consequently, if  $P_{k+1} B_k Q_k^T$  is a near best rank  $k$  approximation to



$A$  with an approximate accuracy  $\sigma_{k+1}$  and the  $k$  singular values of  $B_k$  approximate the first  $k$  large ones of  $A$  in natural order for  $k \leq k_0$ , then LSQR and the TSVD method are related naturally and closely because (i)  $x_k^{tsvd}$  and  $x_k^{lsqr}$  are the solutions to the two perturbed problems of (1.1) that replace  $A$  by its two rank  $k$  approximations with the same quality, respectively; (ii)  $x_k^{tsvd}$  and  $x_k^{lsqr}$  solve the two essentially same regularization problems (1.9) and (2.7), respectively. As a consequence, the LSQR iterate  $x_{k_0}^{lsqr}$  is as accurate as  $x_{k_0}^{tsvd}$ , and LSQR has the full regularization. Therefore, that the  $P_{k+1}B_kQ_k^T$  are near best rank  $k$  approximations to  $A$  and the  $k$  singular values of  $B_k$  approximate the large ones of  $A$  in natural order for  $k = 1, 2, \dots, k_0$  are sufficient conditions for which LSQR has the full regularization.

However, we *must remind* that the near best rank  $k$  approximations and the approximations of the singular values of  $B_k$  to the large singular values  $\sigma_i$  in natural order are *not necessary* conditions for the full regularization of LSQR. It is well possible that LSQR has the full regularization even though these conditions are not satisfied, as will be confirmed numerically later.

**3. An elementary analysis on the regularizing effects of LSQR.** The following result (cf., e.g., van der Sluis and van der Vorst [84]) has been widely used, e.g., in Hansen [36], to illustrate the regularizing effects of LSQR and CGLS.

PROPOSITION 3.1. *LSQR applied to (1.1) with the starting vector  $p_1 = b/\|b\|$  and CGLS applied to  $A^T A x = A^T b$  with the zero starting vector generate the same iterates*

$$(3.1) \quad x_k^{lsqr} = \sum_{i=1}^n f_i^{(k)} \frac{u_i^T b}{\sigma_i} v_i, \quad k = 1, 2, \dots, n,$$

where the filters

$$(3.2) \quad f_i^{(k)} = 1 - \prod_{j=1}^k \frac{(\theta_j^{(k)})^2 - \sigma_i^2}{(\theta_j^{(k)})^2}, \quad i = 1, 2, \dots, n,$$

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

This proposition shows that  $x_k^{lsqr}$  has a filtered SVD expansion. It is easily justified that if the  $k$  Ritz values  $\theta_j^{(k)}$  approximate the first  $k$  singular values  $\sigma_j$  of  $A$  in natural order then the filters  $f_i^{(k)} \approx 1$  for  $i = 1, 2, \dots, k$  and  $f_i^{(k)}$  monotonically approach zero for  $i = k+1, \dots, n$ . This indicates that if the  $\theta_j^{(k)}$  approximate the first  $k$  singular values  $\sigma_j$  of  $A$  in natural order for  $k = 1, 2, \dots, k_0$  then LSQR definitely has the full regularization.

Regarding the semi-convergence of LSQR and the TSVD method, we present the following basic result.

THEOREM 3.1. *The semi-convergence of LSQR occurs at some iteration*

$$k^* \leq k_0.$$

*If the Ritz values  $\theta_j^{(k)}$  do not converge to the first  $k$  large singular values  $\sigma_j$  of  $A$  in natural order for some  $k \leq k^*$ , then  $k^* < k_0$ , and vice versa.*

*Proof.* Applying the Cauchy's strict interlacing theorem [80, p.198, Corollary 4.4] to the singular values of  $B_k$  and  $B_n$ , we always have

$$\theta_i^{(k)} < \sigma_i, \quad i = 1, 2, \dots, k.$$



Therefore, at iteration  $k_0 + 1$  one must have  $\theta_{k_0+1}^{(k_0+1)} < \sigma_{k_0+1}$ . As a result, if the  $\theta_i^{(k)}$  approximate the large  $\sigma_i$  in natural order for  $k = 1, 2, \dots, k_0$ , then by (3.1) and (3.2) we have  $f_{k_0+1}^{(k_0+1)} \approx 1$ , meaning that  $x_{k_0+1}^{lsqr}$  must be deteriorated and the semi-convergence of LSQR must occur at iteration  $k^* = k_0$ .

If the  $\theta_j^{(k)}$  do not converge to the large singular values of  $A$  in natural order and  $\theta_k^{(k)} < \sigma_{k_0+1}$  appears for some iteration  $k \leq k_0$  for the first time, then, by the strict interlacing property of singular values of  $B_{k-1}$  and  $B_k$ , it holds that  $\theta_{k-1}^{(k)} > \theta_{k-1}^{(k-1)} > \theta_k^{(k)}$ , meaning that  $\theta_{k-1}^{(k)} > \theta_{k-1}^{(k-1)} > \sigma_{k_0+1}$ . In this case,  $x_k^{lsqr}$  is already deteriorated by the noise  $e$  before iteration  $k$ : Suppose that  $\sigma_{j^*} < \theta_k^{(k)} < \sigma_{k_0+1}$  with  $j^*$  the smallest integer  $j^* > k_0 + 1$ . Then we can easily justify from (3.2) that  $f_i^{(k)} \in (0, 1)$  and tends to zero monotonically for  $i = j^*, j^* + 1, \dots, n$ , but we have

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

since the first factor is non-positive and the second factor is positive by noticing that  $\theta_j^{(k)} > \sigma_i$ ,  $j = 1, 2, \dots, k-1$  for  $i = k_0 + 1, \dots, j^* - 1$ . Hence  $f_i^{(k)} \geq 1$  for  $i = k_0 + 1, \dots, j^* - 1$ , showing that  $x_k^{lsqr}$  has been deteriorated by the noise  $e$  and the semi-convergence of LSQR has occurred at some iteration  $k^* < k_0$ .

On the other hand, if the semi-convergence of LSQR occurs at iteration  $k^* < k_0$ , then the  $k^*$  Ritz values  $\theta_j^{(k^*)}$  must not approximate the first  $k^*$  large singular values  $\sigma_j$  of  $A$  in natural order. Otherwise, notice that  $\theta_{k^*}^{(k^*)} \in (\sigma_{k^*+1}, \sigma_{k^*})$  means  $\theta_{k^*}^{(k^*)} > \sigma_{k^*+1} \geq \sigma_{k_0}$ , which indicates that the semi-convergence of LSQR does not yet occur at iteration  $k^*$ , a contradiction.  $\square$

If the semi-convergence of LSQR occurs at iteration  $k^* < k_0$ , the regularizing effects of LSQR is much more complicated, and there has been no definitive result on the full or partial regularization of LSQR. This problem will be our future concern.

The standard  $k$ -step Lanczos bidiagonalization method [8, 9] computes the  $k$  Ritz values  $\theta_j^{(k)}$ , which is mathematically equivalent to the symmetric Lanczos method for the eigenvalue problem of  $A^T A$  starting with  $q_1 = A^T b / \|A^T b\|$ ; see [2, 8, 9, 72, 86] or [49, 50] for several variations that are based on standard, harmonic, and refined projection [2, 79, 86] or a combination of them [48]. An attractive feature is that, for general singular value distribution and  $b$ , some  $\theta_i^{(k)}$  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, the large  $\theta_j^{(k)}$  converge fast but small  $\theta_j^{(k)}$  show up late and converge slowly.

For (1.1), since the singular values  $\sigma_j$  of  $A$  decay to zero,  $A^T b = \sum_{j=1}^n \sigma_j (u_j^T b) v_j$  contains more information on dominant right singular vectors than on the ones corresponding to small singular values. Therefore, the Krylov subspace  $\mathcal{V}_k^R$  with  $A^T b$  as the starting vector is expected to contain richer information on the first  $k$  right singular vectors  $v_j$  than on the other  $n - k$  ones. In the meantime, notice that  $A$  has many small singular values clustered at zero. Due to these two basic facts, all the  $\theta_j^{(k)}$  are expected to approximate the large singular values of  $A$  in natural order until some iteration  $k$ . In this case, the iterates  $x_k^{lsqr}$  mainly consists of the  $k$  dominant SVD components of  $A$ . This is why LSQR and CGLS have general regularizing effects; see, e.g., [1, 36, 38, 39].

Unfortunately, the above arguments are purely qualitative and not rigorous. They do not give any hints on the size of  $k$  for possible desired convergence in natural order for any given (1.1). As has been addressed previously, proving how the Ritz values converge is extremely difficult.

**4. The  $\sin \Theta$  theorem and its estimates for the 2-norm distances between  $\mathcal{V}_k^R$  and  $\mathcal{V}_k$ .** As can be seen from Sections 2–3, a complete understanding of the regularization of LSQR includes accurate solutions of the following problems: (i) How accurately does the  $k$  dimensional right Krylov subspace  $\mathcal{V}_k^R$  approximate the  $k$  dimensional dominant right singular subspace  $\mathcal{V}_k$  of  $A$ ? (ii) How accurate is the rank  $k$  approximation  $P_{k+1}B_kQ_k^T$  to  $A$ ? (iii) When do the  $\theta_j^{(k)}$  approximate the large  $\sigma_j$  in natural order? (iv) When does at least a small Ritz value appear, i.e.,  $\theta_k^{(k)} < \sigma_{k+1}$  for some  $k \leq k^*$ ? (v) Does LSQR have the full or partial regularization when the  $k$  Ritz values  $\theta_j^{(k)}$  do not approximate the large  $\sigma_j$  in natural order for some  $k \leq k^*$ ? (vi) What are the counterparts of Problems (i)–(v) in the case that  $A$  has multiple singular values, and what are the accurate solutions or definitive answers correspondingly?

Problem (i) is the starting and key point of the other problems, and its accurate solutions form an absolutely necessary basis of dealing with the others. In this paper, we focus on Problem (i) and present accurate results for the three kinds of ill-posed problems. By them, we will make an elementary exploration on Problem (iv). In-depth treatments of Problem (iv) and the others will given in separate papers.

In terms of the canonical angles  $\Theta(\mathcal{X}, \mathcal{Y})$  between two subspaces  $\mathcal{X}$  and  $\mathcal{Y}$  of equal dimension (cf. [79, p.74–5] and [80, p.43]), we first present a general  $\sin \Theta$  theorem which measures the 2-norm distance between  $\mathcal{V}_k^R$  and  $\mathcal{V}_k$ .

LEMMA 4.1. *For  $k = 1, 2, \dots, n-1$  we have*

$$(4.1) \quad \|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| = \frac{\|\Delta_k\|}{\sqrt{1 + \|\Delta_k\|^2}}$$

with  $\Delta_k \in \mathbb{R}^{(n-k) \times k}$  defined by (4.4).

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

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

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

$$(4.2) \quad D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix}, \quad T_k = \begin{pmatrix} T_{k1} \\ T_{k2} \end{pmatrix},$$

where  $D_1, T_{k1} \in \mathbb{R}^{k \times k}$ . Since  $T_{k1}$  is a Vandermonde matrix with  $\sigma_j$  distinct for  $j = 1, 2, \dots, k$ , it is nonsingular. Therefore, from  $\mathcal{K}_k(A^T A, A^T b) = \text{span}\{VDT_k\}$  we have

$$(4.3) \quad \mathcal{V}_k^R = \mathcal{K}_k(A^T A, A^T b) = \text{span} \left\{ V \begin{pmatrix} D_1 T_{k1} \\ D_2 T_{k2} \end{pmatrix} \right\} = \text{span} \left\{ V \begin{pmatrix} I \\ \Delta_k \end{pmatrix} \right\},$$

where

$$(4.4) \quad \Delta_k = D_2 T_{k2} T_{k1}^{-1} D_1^{-1} \in \mathbb{R}^{(n-k) \times k}.$$

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

$$(4.5) \quad Z_k = V \begin{pmatrix} I \\ \Delta_k \end{pmatrix} = V_k + V_k^\perp \Delta_k.$$

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  $\mathcal{V}_k^R$ . As a result, from (4.5) we get an orthogonal direct sum decomposition

$$(4.6) \quad \hat{Z}_k = (V_k + V_k^\perp \Delta_k)(I + \Delta_k^T \Delta_k)^{-\frac{1}{2}}.$$

By the definition of  $\Theta(\mathcal{V}_k, \mathcal{V}_k^R)$  and (4.6), we obtain

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

which proves (4.1).  $\square$

We remark that it is direct from (4.1) to get

$$(4.7) \quad \|\tan \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| = \|\Delta_k\|.$$

(4.1) has been established in [46, Theorem 2.1], and we include the proof here for completeness and for the introduction of notation  $\|\Delta_k\|$ , which will be used later.

We now establish accurate estimates for  $\|\Delta_k\|$  for severely ill-posed problems.

**THEOREM 4.2.** *Let the SVD of  $A$  be as (1.5), and assume that (1.1) is severely ill-posed with  $\sigma_j = \mathcal{O}(\rho^{-j})$  and  $\rho > 1$ ,  $j = 1, 2, \dots, n$ . Then*

$$(4.8) \quad \|\Delta_1\| \leq \frac{\sigma_2 \max_{2 \leq i \leq n} |u_i^T b|}{\sigma_1 |u_1^T b|} (1 + \mathcal{O}(\rho^{-2})),$$

$$(4.9) \quad \|\Delta_k\| \leq \frac{\sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b|}{\sigma_k \min_{1 \leq i \leq k} |u_i^T b|} (1 + \mathcal{O}(\rho^{-2})) |L_{k_1}^{(k)}(0)|, \quad k = 2, 3, \dots, n-1,$$

where

$$(4.10) \quad |L_{k_1}^{(k)}(0)| = \max_{j=1,2,\dots,k} |L_j^{(k)}(0)|, \quad |L_j^{(k)}(0)| = \prod_{i=1, i \neq j}^k \frac{\sigma_i^2}{|\sigma_j^2 - \sigma_i^2|}, \quad j = 1, 2, \dots, k.$$

*Proof.* For  $k = 2, 3, \dots, n-1$ , it is easily justified that the  $j$ -th column of  $T_{k_1}^{-1}$  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  $T_{k_2} T_{k_1}^{-1}$  is

$$(4.11) \quad T_{k_2} T_{k_1}^{-1} e_j^{(k)} = (L_j^{(k)}(\sigma_{k+1}^2), \dots, L_j^{(k)}(\sigma_n^2))^T, \quad j = 1, 2, \dots, k,$$

from which we obtain

$$(4.12) \quad T_{k_2} T_{k_1}^{-1} = \begin{pmatrix} L_1^{(k)}(\sigma_{k+1}^2) & L_2^{(k)}(\sigma_{k+1}^2) & \dots & L_k^{(k)}(\sigma_{k+1}^2) \\ L_1^{(k)}(\sigma_{k+2}^2) & L_2^{(k)}(\sigma_{k+2}^2) & \dots & L_k^{(k)}(\sigma_{k+2}^2) \\ \vdots & \vdots & \ddots & \vdots \\ L_1^{(k)}(\sigma_n^2) & L_2^{(k)}(\sigma_n^2) & \dots & L_k^{(k)}(\sigma_n^2) \end{pmatrix} \in \mathbb{R}^{(n-k) \times k}.$$

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

$$\begin{aligned}
 |\Delta_k| &= |D_2 T_{k_2} T_{k_1}^{-1} D_1^{-1}| \\
 &\leq \begin{pmatrix} \frac{\sigma_{k+1}}{\sigma_1} \left| \frac{u_{k+1}^T b}{u_1^T b} \right| |L_{k_1}^{(k)}(0)| & \frac{\sigma_{k+1}}{\sigma_2} \left| \frac{u_{k+1}^T b}{u_2^T b} \right| |L_{k_1}^{(k)}(0)| & \dots & \frac{\sigma_{k+1}}{\sigma_k} \left| \frac{u_{k+1}^T b}{u_k^T b} \right| |L_{k_1}^{(k)}(0)| \\ \frac{\sigma_{k+2}}{\sigma_1} \left| \frac{u_{k+2}^T b}{u_1^T b} \right| |L_{k_1}^{(k)}(0)| & \frac{\sigma_{k+2}}{\sigma_2} \left| \frac{u_{k+2}^T b}{u_2^T b} \right| |L_{k_1}^{(k)}(0)| & \dots & \frac{\sigma_{k+2}}{\sigma_k} \left| \frac{u_{k+2}^T b}{u_k^T b} \right| |L_{k_1}^{(k)}(0)| \\ \vdots & \vdots & & \vdots \\ \frac{\sigma_n}{\sigma_1} \left| \frac{u_n^T b}{u_1^T b} \right| |L_{k_1}^{(k)}(0)| & \frac{\sigma_n}{\sigma_2} \left| \frac{u_n^T b}{u_2^T b} \right| |L_{k_1}^{(k)}(0)| & \dots & \frac{\sigma_n}{\sigma_k} \left| \frac{u_n^T b}{u_k^T b} \right| |L_{k_1}^{(k)}(0)| \end{pmatrix} \\
 (4.13) \quad &= |L_{k_1}^{(k)}(0)| |\tilde{\Delta}_k|,
 \end{aligned}$$

where

$$(4.14) \quad |\tilde{\Delta}_k| = \left| (\sigma_{k+1} u_{k+1}^T b, \sigma_{k+2} u_{k+2}^T b, \dots, \sigma_n u_n^T b)^T \left( \frac{1}{\sigma_1 u_1^T b}, \frac{1}{\sigma_2 u_2^T b}, \dots, \frac{1}{\sigma_k u_k^T b} \right) \right|$$

is a rank one matrix. Therefore, by  $\|C\| \leq \|C\|$  (cf. [78, p.53]), we have

$$\begin{aligned}
 \|\Delta_k\| &\leq \| |\Delta_k| \| \leq |L_{k_1}^{(k)}(0)| \|\tilde{\Delta}_k\| \\
 (4.15) \quad &= |L_{k_1}^{(k)}(0)| \left( \sum_{j=k+1}^n \sigma_j^2 |u_j^T b|^2 \right)^{1/2} \left( \sum_{j=1}^k \frac{1}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2}.
 \end{aligned}$$

In the following we bound the above two square root factors separately.

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

$$\begin{aligned}
 \left( \sum_{j=k+1}^n \sigma_j^2 |u_j^T b|^2 \right)^{1/2} &= \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| \left( \sum_{j=k+1}^n \frac{\sigma_j^2 |u_j^T b|^2}{\sigma_{k+1}^2 \max_{k+1 \leq i \leq n} |u_i^T b|} \right)^{1/2} \\
 &\leq \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| \left( \sum_{j=k+1}^n \frac{\sigma_j^2}{\sigma_{k+1}^2} \right)^{1/2} \\
 &= \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| \left( 1 + \sum_{j=k+2}^n \mathcal{O}(\rho^{2(k-j)+2}) \right)^{1/2} \\
 &= \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| \left( 1 + \mathcal{O} \left( \sum_{j=k+2}^n \rho^{2(k-j)+2} \right) \right)^{1/2} \\
 &= \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| \left( 1 + \mathcal{O} \left( \frac{\rho^{-2}}{1 - \rho^{-2}} (1 - \rho^{-2(n-k-1)}) \right) \right)^{1/2} \\
 &= \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| (1 + \mathcal{O}(\rho^{-2}))^{1/2} \\
 (4.16) \quad &= \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| (1 + \mathcal{O}(\rho^{-2}))
 \end{aligned}$$

with  $1 + \mathcal{O}(\rho^{-2}) = 1$  for  $k = n - 1$ .

For  $k = 2, 3, \dots, n - 1$ , we get

$$\begin{aligned}
\left( \sum_{j=1}^k \frac{1}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2} &= \frac{1}{\sigma_k \min_{1 \leq i \leq k} |u_i^T b|} \left( \sum_{j=1}^k \frac{\sigma_k^2 \min_{1 \leq i \leq k} |u_i^T b|}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2} \\
&\leq \frac{1}{\sigma_k \min_{1 \leq i \leq k} |u_i^T b|} \left( \sum_{j=1}^k \frac{\sigma_k^2}{\sigma_j^2} \right)^{1/2} \\
&= \frac{1}{\sigma_k \min_{1 \leq i \leq k} |u_i^T b|} \left( 1 + \mathcal{O} \left( \sum_{j=1}^{k-1} \rho^{2(j-k)} \right) \right)^{1/2} \\
&= \frac{1}{\sigma_k \min_{1 \leq i \leq k} |u_i^T b|} (1 + \mathcal{O}(\rho^{-2})).
\end{aligned}$$

From the above and (4.15)–(4.16), we finally obtain (4.9).

Note that the Lagrange polynomials  $L_j^{(k)}(\lambda)$  require  $k \geq 2$ . Therefore, we need to treat the case  $k = 1$  separately. Note that

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

Therefore, from (4.4) we have

$$(4.17) \quad \Delta_1 = (\sigma_2 u_2^T b, \sigma_3 u_3^T b, \dots, \sigma_n u_n^T b)^T \frac{1}{\sigma_1 u_1^T b},$$

from which and (4.16) it is direct to get (4.8).  $\square$

A crucial step in proving (4.8)–(4.10) is to first derive (4.13)–(4.14) and then bound the resulting *rank one* matrix accurately. Huang and Jia [46] simply bounded

$$\|\Delta_k\| \leq \|\Delta_k\|_F \leq \|D_2\| \|T_{k2} T_{k1}^{-1}\|_F \|D_1^{-1}\|$$

with  $\|\cdot\|_F$  the F-norm of a matrix, which led to a too pessimistic overestimate

$$\|\Delta_k\| \leq \frac{\sigma_{k+1}}{\sigma_k} \frac{\max_{k+1 \leq i \leq n} |u_i^T b|}{\min_{1 \leq i \leq k} |u_i^T b|} \sqrt{k(n-k)} |L_{k1}^{(k)}(0)|$$

due to the excessive factor  $\sqrt{k(n-k)}$ , which ranges from  $\sqrt{n-1}$  to  $\frac{n}{2}$  for  $n$  even and  $\frac{\sqrt{n^2-1}}{2}$  for  $n$  odd.

$\|\Delta_k\|$  and  $|L_j^{(k)}(0)|$ ,  $j = 1, 2, \dots, k$  are used to study the regularizing effects of LSQR in [36, p.150-2], but there have been no estimates on them for any kind of ill-posed problem. We next give accurate estimates for  $|L_j^{(k)}(0)|$ ,  $j = 1, 2, \dots, k$  and get insight into them for severely ill-posed problems.

**THEOREM 4.3.** *For the severely ill-posed problem with the singular values  $\sigma_j =$*

$\mathcal{O}(\rho^{-j})$  and suitable  $\rho > 1$ ,  $j = 1, 2, \dots, n$  and  $k = 2, 3, \dots, n-1$ , we have

$$(4.18) \quad |L_k^{(k)}(0)| = 1 + \mathcal{O}(\rho^{-2}),$$

$$(4.19) \quad |L_j^{(k)}(0)| = \frac{1 + \mathcal{O}(\rho^{-2})}{\prod_{i=j+1}^k \left(\frac{\sigma_i}{\sigma_j}\right)^2} = \frac{1 + \mathcal{O}(\rho^{-2})}{\mathcal{O}(\rho^{(k-j)(k-j+1)})}, \quad j = 1, 2, \dots, k-1,$$

$$(4.20) \quad |L_{k_1}^{(k)}(0)| = \max_{j=1,2,\dots,k} |L_j^{(k)}(0)| = 1 + \mathcal{O}(\rho^{-2}).$$

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

$$(4.21) \quad \begin{aligned} |L_j^{(k)}(0)| &= \prod_{i=1, i \neq j}^k \left| \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} \right| = \prod_{i=1}^{j-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} \cdot \prod_{i=j+1}^k \frac{\sigma_i^2}{\sigma_j^2 - \sigma_i^2} \\ &= \prod_{i=1}^{j-1} \frac{1}{1 - \mathcal{O}(\rho^{-2(j-i)})} \prod_{i=j+1}^k \frac{1}{1 - \mathcal{O}(\rho^{-2(i-j)})} \frac{1}{\prod_{i=j+1}^k \mathcal{O}(\rho^{2(i-j)})} \\ &= \frac{\left(1 + \sum_{i=1}^j \mathcal{O}(\rho^{-2i})\right) \left(1 + \sum_{i=1}^{k-j+1} \mathcal{O}(\rho^{-2i})\right)}{\prod_{i=j+1}^k \mathcal{O}(\rho^{2(i-j)})} \end{aligned}$$

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

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

which proves (4.18).

For the numerator of (4.21) we have

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

and

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

whose product for any  $k$  is

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

On the other hand, note that the denominator of (4.21) is defined by

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

which, together with the above estimate for the numerator of (4.21), proves (4.19). Since the above quantity is always *bigger than one* for  $j = 1, 2, \dots, k-1$ , for any  $k$ , combining (4.18) with (4.19) gives (4.20).  $\square$

REMARK 4.1. (4.20) indicates that the bounds (4.8) and (4.9) can be unified as

$$(4.22) \quad \|\Delta_k\| \leq \frac{\sigma_{k+1}}{\sigma_k} \frac{\max_{k+1 \leq i \leq n} |u_i^T b|}{\min_{1 \leq i \leq k} |u_i^T b|} (1 + \mathcal{O}(\rho^{-2})), \quad k = 1, 2, \dots, n-1.$$

REMARK 4.2. (i) (4.19) shows that  $|L_j^{(k)}(0)|$  exhibits monotonic increasing property with  $j$  for a fixed  $k$ , and  $k_1$  in (4.20) is close to  $k$ ; (ii)  $|L_j^{(k)}(0)|$  decays monotonically with  $k$  for a fixed  $j$ ; (iii) (4.20) indicates  $|L_{k_1}^{(k)}(0)|$  almost remains a constant close to one with  $k$  for suitable  $\rho > 1$ .

By taking the equalities in (4.8) and (4.9) as estimates for  $\|\Delta_k\|$ , we substitute them into (4.1) and compute the corresponding estimates for  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$ . We next illustrate the sharpness of our estimates and justify Remark 4.2.

Before proceeding, we make some necessary comments. By the discrete Picard condition (1.7), (1.8) and the properties of  $e$ , it is known from [36, p.70-1] and [39, p.41-2] that  $|u_j^T b| \approx |u_j^T b_{true}| = \sigma_j^{1+\beta} > \eta$  monotonically decreases with  $j = 1, 2, \dots, k_0$ , and  $|u_j^T b| \approx |u_j^T e|$  with the expected values  $\mathcal{E}(|u_j^T e|) = \eta$  for  $j > k_0$ . Therefore, we must have

$$(4.23) \quad \frac{\max_{k+1 \leq i \leq n} |u_i^T b|}{\min_{1 \leq i \leq k} |u_i^T b|} \approx \frac{|u_{k+1}^T b|}{|u_k^T b|} \approx \frac{\sigma_{k+1}^{1+\beta}}{\sigma_k^{1+\beta}} < 1, \quad k = 1, 2, \dots, k_0,$$

$$(4.24) \quad \frac{\max_{k+1 \leq i \leq n} |u_i^T b|}{\min_{1 \leq i \leq k} |u_i^T b|} \approx \frac{|u_{k+1}^T b|}{|u_k^T b|} \approx \frac{\eta}{\eta} = 1, \quad k = k_0 + 1, \dots, n-1.$$

In numerical justifications, we will use  $\frac{|u_{k+1}^T b|}{|u_k^T b|}$  to replace the left-hand sides of (4.23) and (4.24). It is known from [79, 80] that if the ratio  $\sigma_1/\sigma_k = \mathcal{O}(\frac{1}{\epsilon_{\text{mach}}})$  then both  $\sigma_k$  and  $(u_k, v_k)$  are generally computed with no accuracy in finite precision arithmetic, where  $\epsilon_{\text{mach}} = 2.22 \times 10^{-16}$  is the machine precision, since  $\sigma_k$  is very close to its neighbors for ill-posed problems. Thus, our above treatment is not only reasonable but also avoids the *intrinsic* difficulty to accurately compute the left-hand sides of (4.23) and (4.24) which involve all the left singular vectors, including those associated with small singular values clustered at zero that are computed with no accuracy.

In the meantime, the above also tells us that it is *unreliable* to compute  $\Delta_k$  defined by (4.4) and  $\|\Delta_k\|$  because, in finite precision arithmetic, we cannot compute  $T_{k2}$  in (4.2) reliably due to the high inaccuracy of the computed small singular values and the possible underflows of  $\sigma_i^{2j-2}$  for  $i$  big and  $j = 1, 2, \dots, k$ . Fortunately, we can use the Matlab built-in function `subspace.m`, which computes the maximum of the canonical angles  $\Theta(\mathcal{V}_k, \mathcal{V}_k^R)$ , to calculate  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  accurately when the first  $k$  singular triplets  $(\sigma_i, u_i, v_i)$  are computed accurately.

It appears hard to find a 2D real-life severely ill-posed problem for justifying the sharpness of our estimates in Theorems 4.2–4.3. Gazzola, Hansen and Nagy [21] have



very recently presented a number of 2D test problems, where the image deblurring problem **PRblurgauss**, the inverse diffusion problem **PRdiffusion** and the nuclear magnetic resonance (NMR) relaxometry problem **PRnmr** are severely ill-posed. But the latter two matrices are only available as a function handle, for which we cannot compute their SVDs. Setting the parameter `options.BlurLevel='severe'`, we have computed the SVD of **PRblurgauss** with  $m = n = 10000$  and found  $\sigma_1/\sigma_{1500} \approx 1.99 \times 10^{14} = \mathcal{O}(\frac{1}{\epsilon_{\text{mach}}})$ . Unfortunately, we have found out that at least half of the first 1500 singular values are (genuinely or at least numerically) *multiple*. For example, among the first 40 singular values,  $\sigma_3, \sigma_6, \sigma_8, \sigma_{11}, \sigma_{13}, \sigma_{15}, \sigma_{17}, \sigma_{19}, \sigma_{22}, \sigma_{24}, \sigma_{25}, \sigma_{26}, \sigma_{28}, \sigma_{30}, \sigma_{33}, \sigma_{35}, \sigma_{37}$  and  $\sigma_{39}$  are multiple. As a result, Theorems 4.2–4.3 cannot apply here because of multiple singular values. In addition, we have found that the average decay rate of the *distinct* ones among the first 1500 singular value is approximately  $\rho^{-1} = 0.9697$ , i.e.,  $\rho = 1.0312$ , which is *fairly* close to one and means that the problem is only *slightly* severely ill-posed.

We should point out that, for the purpose of justifying the sharpness of our estimates in Theorems 4.2–4.3, it is enough to test any severely ill-posed problem with the discrete Picard condition satisfied. To this end, we take the 1D severely ill-posed problem **shaw** of  $m = n = 10240$  from [37] with  $\sigma_k = \mathcal{O}(e^{-2k})$ , where  $e$  is the natural constant. We take  $\rho = e^2$ , and compute the estimate (4.1) for  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  by taking the equalities in (4.8) and (4.9),  $1 + \mathcal{O}(\rho^{-2}) = 1 + 2\rho^{-2}$  and  $(1 + \mathcal{O}(\rho^{-2})) |L_{k_1}^{(k)}(0)| = 1 + 3\rho^{-2}$ . For  $k > 1$ , we use (4.10) to compute  $|L_j^{(k)}(0)|$ ,  $j = 1, 2, \dots, k$  and  $|L_{k_1}^{(k)}(0)|$  so as to confirm Theorem 4.3 and Remark 4.2. We generate  $b = b_{\text{true}} + e$  with  $\varepsilon = \frac{\|e\|}{\|b_{\text{true}}\|} = 10^{-3}$  and  $e$  the Gaussian white noise with zero mean. In all the figures, we will abbreviate  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  by  $\sin \Theta_k$ .

Figure 1 (a) plots the first 40 singular values  $\sigma_k$  of **shaw**, and we find  $\sigma_1/\sigma_{21} \approx 2.4 \times 10^{15} = \mathcal{O}(\frac{1}{\epsilon_{\text{mach}}})$ , meaning that the  $(\sigma_k, u_k, v_k)$  are generally computed with no accuracy for  $k \geq 21$ . Figure 1 (b) clearly confirms each of the three points in Remark 4.2. Moreover, we see that the  $|L_j^{(k)}(0)|$  become tiny swiftly for  $j$  small when  $k$  increases. Figure 1 (c) indicates that our estimates for  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  match the exact ones quite well for  $k = 1, 2, \dots, 15$ . We have found that the maximum and minimum of ratios of the estimated and exact ones are 1.3924 and 0.7485, respectively, and the geometric mean of these ratios is 0.9146. Precisely, the fifteen ratios are 0.9386, 0.9924, 0.8564, 1.0382, 1.1781, 1.0719, 1.0851, 1.0302, 1.2323, 1.3630, 0.7485, 1.0624, 1.3013, 1.3488, 1.3924, respectively. Figure 1 (d) draws the semi-convergence process of LSQR and the TSVD method. It shows that they compute the best regularized solutions at the same iterations  $k^* = k_0 = 9$  and the best LSQR solution  $x_{k^*}^{\text{lsqr}}$  is as accurate as the best TSVD solution  $x_{k_0}^{\text{tsvd}}$ .

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

**THEOREM 4.4.** *For a moderately or mildly ill-posed (1.1) with the singular values  $\sigma_j = \zeta j^{-\alpha}$ ,  $j = 1, 2, \dots, n$ , where  $\alpha > \frac{1}{2}$  and  $\zeta > 0$  is some constant, we have*

$$(4.25) \quad \|\Delta_1\| \leq \frac{\max_{2 \leq i \leq n} |u_i^T b|}{|u_1^T b|} \sqrt{\frac{1}{2\alpha - 1}},$$

$$(4.26) \quad \|\Delta_k\| \leq \frac{\max_{k+1 \leq i \leq n} |u_i^T b|}{\min_{1 \leq i \leq k} |u_i^T b|} \sqrt{\frac{k^2}{4\alpha^2 - 1} + \frac{k}{2\alpha - 1}} |L_{k_1}^{(k)}(0)|, \quad k = 2, 3, \dots, n-1.$$

*Proof.* We only need to accurately bound the right-hand side of (4.15). For

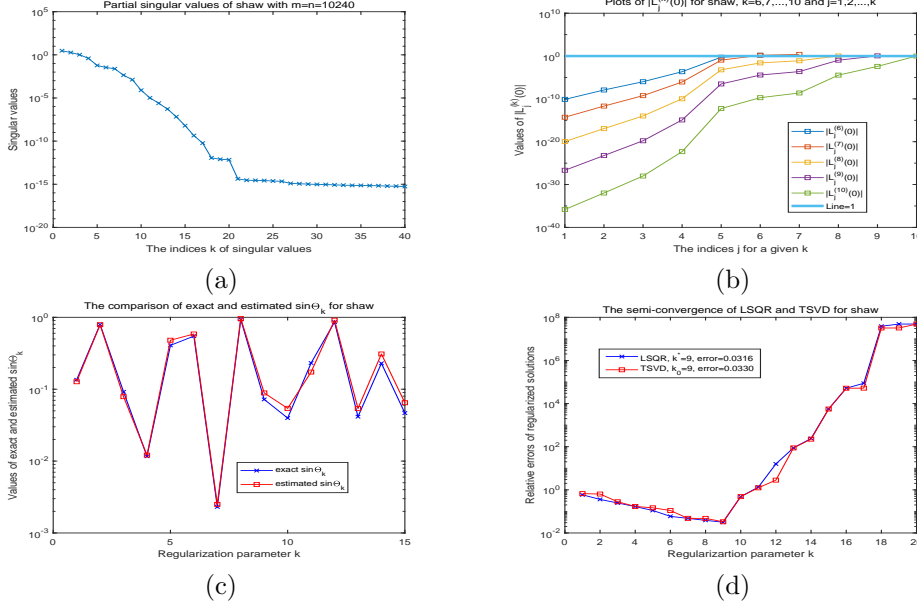


FIG. 1. (a): Partial singular values of shaw; (b): plots of  $|L_j^{(k)}(0)|$  for  $k = 6, 7, 8, 9, 10$ ; (c): the exact and estimated  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$ ; (d): the semi-convergence process of LSQR and TSVD.

$k = 1, 2, \dots, n-1$ , we obtain

$$\begin{aligned}
 \left( \sum_{j=k+1}^n \sigma_j^2 |u_j^T b|^2 \right)^{1/2} &= \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| \left( \sum_{j=k+1}^n \frac{\sigma_j^2 |u_j^T b|^2}{\sigma_{k+1}^2 \max_{k+1 \leq i \leq n} |u_i^T b|^2} \right)^{1/2} \\
 &\leq \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| \left( \sum_{j=k+1}^n \frac{\sigma_j^2}{\sigma_{k+1}^2} \right)^{1/2} \\
 &= \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| \left( \sum_{j=k+1}^n \left( \frac{j}{k+1} \right)^{-2\alpha} \right)^{1/2} \\
 &= \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| \left( (k+1)^{2\alpha} \sum_{j=k+1}^n \frac{1}{j^{2\alpha}} \right)^{1/2} \\
 &< \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| (k+1)^\alpha \left( \int_k^\infty \frac{1}{x^{2\alpha}} dx \right)^{1/2} \\
 &= \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| \left( \frac{k+1}{k} \right)^\alpha \sqrt{\frac{k}{2\alpha-1}} \\
 &= \sigma_{k+1} \max_{k+1 \leq i \leq n} |u_i^T b| \frac{\sigma_k}{\sigma_{k+1}} \sqrt{\frac{k}{2\alpha-1}} \\
 (4.27) \quad &= \sigma_k \max_{k+1 \leq i \leq n} |u_i^T b| \sqrt{\frac{k}{2\alpha-1}}.
 \end{aligned}$$

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

$$\begin{aligned}
 \left( \sum_{j=1}^k \frac{1}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2} &= \frac{1}{\sigma_k \min_{1 \leq i \leq k} |u_i^T b|} \left( \sum_{j=1}^k \frac{\sigma_k^2 \min_{1 \leq i \leq k} |u_i^T b|^2}{\sigma_j^2 |u_j^T b|^2} \right)^{1/2} \\
 &\leq \frac{1}{\sigma_k \min_{1 \leq i \leq k} |u_i^T b|} \left( \sum_{j=1}^k \frac{\sigma_k^2}{\sigma_j^2} \right)^{1/2} \\
 &= \frac{1}{\sigma_k \min_{1 \leq i \leq k} |u_i^T b|} \left( \sum_{j=1}^k \left( \frac{j}{k} \right)^{2\alpha} \right)^{1/2} \\
 &= \frac{1}{\sigma_k \min_{1 \leq i \leq k} |u_i^T b|} \left( k \sum_{j=1}^k \frac{1}{k} \left( \frac{j-1}{k} \right)^{2\alpha} + 1 \right)^{1/2} \\
 &< \frac{1}{\sigma_k \min_{1 \leq i \leq k} |u_i^T b|} \left( k \int_0^1 x^{2\alpha} dx + 1 \right)^{1/2} \\
 (4.28) \quad &\leq \frac{1}{\sigma_k \min_{1 \leq i \leq k} |u_i^T b|} \sqrt{\frac{k}{2\alpha+1} + 1}.
 \end{aligned}$$

Substituting the above and (4.27) into (4.15) yields (4.26). For  $k = 1$ , (4.25) follows from (4.17) and (4.27).  $\square$

REMARK 4.3. *For a purely technical reason, we have used the simplifying singular value model  $\sigma_j = \zeta j^{-\alpha}$  to replace the general form  $\sigma_j = \mathcal{O}(j^{-\alpha})$ . This simplifying model can avoid some troublesome derivations and non-transparent formulations.*

In the following we estimate  $|L_j^{(k)}(0)|, j = 1, 2, \dots, k$  for moderately and mildly ill-posed problems. As will be seen from the proof, it turns out impossible to bound them from above both elegantly and accurately unless  $\alpha > 1$  sufficiently.

THEOREM 4.5. *For a moderately ill-posed problem with  $\sigma_j = \zeta j^{-\alpha}, j = 1, 2, \dots, n$  and  $\alpha > 1$ , if  $\alpha > 1$  suitably, then for  $k = 2, 3, \dots, n-1$  we have*

$$(4.29) \quad |L_j^{(k)}(0)| \approx \left( 1 + \frac{j}{2\alpha+1} \right) \prod_{i=j+1}^k \left( \frac{j}{i} \right)^{2\alpha}, \quad j = 1, 2, \dots, k-1,$$

$$(4.30) \quad \frac{k}{2\alpha+1} < |L_{k_1}^{(k)}(0)| \approx 1 + \frac{k}{2\alpha+1}$$

with the lower bound requiring that  $k$  satisfies  $\frac{2\alpha+1}{k} \leq 1$ ; for a mildly ill-posed problem with  $\sigma_j = \zeta j^{-\alpha}, j = 1, 2, \dots, n$  and  $\frac{1}{2} < \alpha \leq 1$ , if  $k$  satisfies  $\frac{2\alpha+1}{k} \leq 1$ , we have

$$(4.31) \quad \frac{k}{2\alpha+1} < |L_{k_1}^{(k)}(0)|.$$

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

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

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

$$\begin{aligned}
 |L_j^{(k)}(0)| &= \prod_{i=1, i \neq j}^k \left| \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} \right| = \prod_{i=1}^{j-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_j^2} \cdot \prod_{i=j+1}^k \frac{\sigma_i^2}{\sigma_j^2 - \sigma_i^2} \\
 &= \prod_{i=1}^{j-1} \frac{1}{1 - \left(\frac{i}{j}\right)^{2\alpha}} \prod_{i=j+1}^k \frac{1}{1 - \left(\frac{j}{i}\right)^{2\alpha}} \frac{1}{\prod_{i=j+1}^k \left(\frac{i}{j}\right)^{2\alpha}} \\
 &\approx \left(1 + \sum_{i=1}^{j-1} \left(\frac{i}{j}\right)^{2\alpha}\right) \left(1 + \sum_{i=j+1}^k \left(\frac{j}{i}\right)^{2\alpha}\right) \prod_{i=j+1}^k \left(\frac{j}{i}\right)^{2\alpha} \\
 &\leq \left(1 + \int_0^1 x^{2\alpha} dx\right) \left(1 + j^{2\alpha} \int_j^k \frac{1}{x^{2\alpha}} dx\right) \prod_{i=j+1}^k \left(\frac{j}{i}\right)^{2\alpha} \\
 &= \left(1 + \frac{j}{2\alpha + 1}\right) \left(1 + \frac{j - j^{2\alpha} k^{-2\alpha+1}}{2\alpha - 1}\right) \prod_{i=j+1}^k \left(\frac{j}{i}\right)^{2\alpha}.
 \end{aligned}$$

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

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

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

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

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

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

which proves (4.29). The right-hand side of (4.30) follows from the monotonic increasing property of the right-hand side of (4.29) with respect to  $j$ .

On the other hand, once  $k$  is such that  $\frac{2\alpha+1}{k} \leq 1$ , we always have

$$\begin{aligned}
 |L_{k_1}^{(k)}(0)| &\geq |L_k^{(k)}(0)| = \prod_{i=1}^{k-1} \frac{\sigma_i^2}{\sigma_i^2 - \sigma_k^2} = \prod_{i=1}^{k-1} \frac{1}{1 - \left(\frac{i}{k}\right)^{2\alpha}} \\
 &> 1 + \sum_{i=1}^{k-1} \left(\frac{i}{k}\right)^{2\alpha} > 1 + k \int_0^{\frac{k-1}{k}} x^{2\alpha} dx \\
 (4.33) \quad &= 1 + \frac{k \left(\frac{k-1}{k}\right)^{2\alpha+1}}{2\alpha+1} \approx 1 + \frac{k}{2\alpha+1} \left(1 - \frac{2\alpha+1}{k}\right) = \frac{k}{2\alpha+1},
 \end{aligned}$$

which yields the lower bound of (4.30) and (4.31).  $\square$

REMARK 4.4. The inaccuracy source of (4.29) and (4.32) consists in using the summations  $1 + \Sigma$  to replace the corresponding products  $\Pi$  in the proof. They are considerable underestimates for  $\frac{1}{2} < \alpha \leq 1$  but are accurate for suitable  $\alpha > 1$ ; the bigger  $\alpha$  is, the more accurate the estimates (4.29) and (4.30) are. The derivation of (4.32) and (4.33) indicates that  $|L_{k_1}^{(k)}(0)|$  is substantially bigger than  $\frac{k}{2\alpha+1}$  and cannot be bounded from above effectively for  $\alpha > \frac{1}{2}$  not big enough.

REMARK 4.5. (4.29) shows that the first two points in Remark 4.2 apply here, and (4.30)–(4.31) indicate that  $|L_{k_1}^{(k)}(0)|$  has increasing tendency with respect to  $k$ .

REMARK 4.6. For severely ill-posed problems, we have  $\frac{\sigma_{k+1}}{\sigma_k} \sim \rho^{-1}$ ,  $\frac{|u_{k+1}^T b|}{|u_k^T b|} \sim \rho^{-1-\beta} < 1$  for  $k \leq k_0$ . Therefore, we see from (4.22)–(4.24) that  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  exhibits neither increasing nor decreasing tendency for  $k = 1, 2, \dots, k_0$  and  $k = k_0 + 1, \dots, n-1$ , respectively, as is numerically justified by Figure 1 (c). However, for moderately ill-posed problems, notice from (1.7) that  $\frac{|u_{k+1}^T b|}{|u_k^T b|} \approx \left(\frac{k}{k+1}\right)^{\alpha(1+\beta)}$  increases slowly; (4.30) indicate that  $\sqrt{\frac{k^2}{4\alpha^2-1} + \frac{k}{2\alpha-1}} |L_{k_1}^{(k)}(0)|$  increases as  $k$  grows. As a result, (4.1) and (4.26) illustrate that  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  exhibits increasing tendency with  $k$ , meaning that  $\mathcal{V}_k^R$  cannot capture  $\mathcal{V}_k$  so well as it does for severely ill-posed problems as  $k$  increases. In fact,  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  starts to approach one as  $k$  increases, meaning that  $\mathcal{V}_k^R$  will contain substantial information on the right singular vectors corresponding to the  $n-k$  small singular values of  $A$ .

REMARK 4.7. Regarding mildly ill-posed problems, (4.33) and the comment on it indicate that  $|L_{k_1}^{(k)}(0)|$  is substantially bigger than one for  $\frac{1}{2} < \alpha \leq 1$ . Consequently, the bound (4.26) thus becomes increasingly large as  $k$  increases, causing that  $\|\Delta_k\|$  is large and  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| \approx 1$  soon.

In the following we justify our results numerically. A number of 2D real-life mildly ill-posed problems are presented in [6, 21, 37], which are from image deblurring, seismic and computerized tomography, inverse diffusion and inverse interpolation, etc. However, we do not find a 2D moderately ill-posed one in [6, 21]. PRblurmotion from [21] is a mildly ill-posed 2D image deblurring problem. We use it to show the effectiveness of our estimates. Taking options.BlurLevel='severe', 'medium', 'mild', we compute the singular values of three corresponding matrices of  $m = n = 10000$ , and find that  $\frac{\sigma_1}{\sigma_n} = 905.3448, 81.1847, 28.7967$ , respectively. In the test, except the matrix order, we take all the other parameters as defaults, by which it is fairly reasonable to use  $\alpha = 0.6$ . We shall illustrate the sharpness of the estimates for (4.1) when inserting (4.25)–(4.26) into it, where we take the equalities in (4.25) and (4.26). As we have commented, since the problem is only mildly ill-posed, we cannot

bound  $|L_{k_1}^{(k)}(0)|$  from above, and instead compute it accurately by definition. We add a Gaussian white noise  $e$  to  $b$  with the relative noise level  $\varepsilon = 0.01$ . Figure 2 plots the results, where Figure 2 (a)–(b) depict the curves of  $|L_j^{(k)}(0)|$  for  $k = 6, 7, 8, 9, 10$  and of  $|L_{k_1}^{(k)}(0)|$  for  $k = 2, 3, \dots, 15$ , respectively, Figure 2 (c) draws the curves of the exact and estimated  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$ , and Figure 2 (d) exhibits the semi-convergence process of LSQR and the TSVD method.

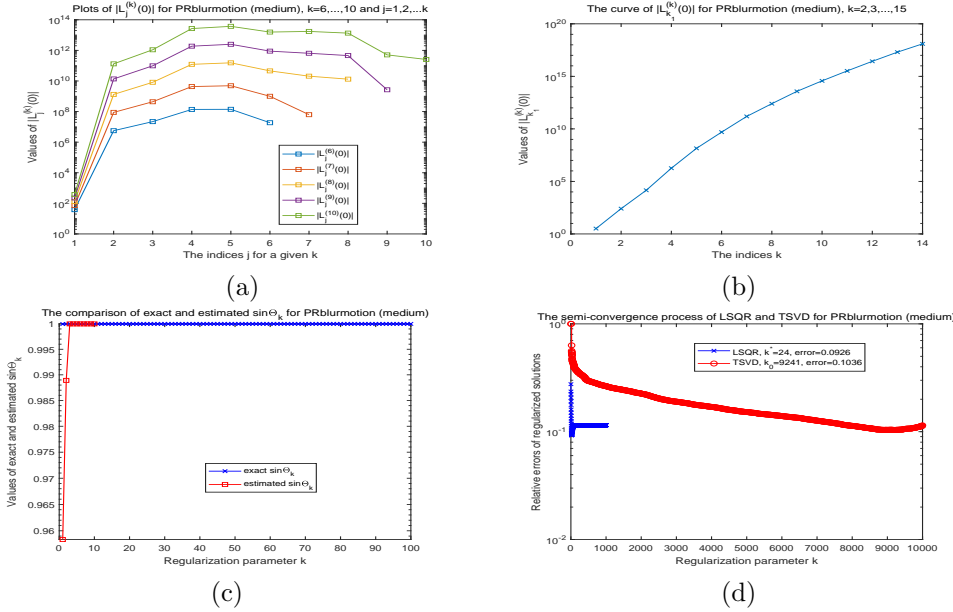


FIG. 2. (a): plots of  $|L_j^{(k)}(0)|$  for  $k = 6, 7, \dots, 10$ ; (b): the curve of  $|L_{k_1}^{(k)}(0)|$  for  $k = 2, 3, \dots, 15$ ; (c): the exact and estimated  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$ ; (d): the semi-convergence process of LSQR and TSVD.

Figure 2 (a) justifies that  $|L_j^{(k)}(0)|$  increases with  $k$  for a fixed  $j$ , and and Figure 2 (b) indicates that  $|L_{k_1}^{(k)}(0)|$  increases very quickly with  $k$ . The ratios of the estimated  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  and true ones are 0.9584, 0.9889, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000, respectively, and the geometric mean is 0.9946. In fact,  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  approaches one from the very first iteration, and the its first four values are 0.999967738200681, 0.999986335237377, 0.999999995155997, 0.99999999987418, respectively, which confirm our theory that  $\mathcal{V}_k^R$  captures  $\mathcal{V}_k$  very poorly and deviates completely from the latter very soon. In any event, however, our estimates for  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  match the true ones very well, as is also seen from Figure 2 (c).

Very surprisingly, for this mildly ill-posed problem, it is completely beyond one's common expectation that the LSQR best solution  $x_{k^*}^{lsqr}$  with the relative error 0.0926 at semi-convergence is at least as accurate as the TSVD best solution  $x_{k_0}^{tsvd}$  with the relative error 0.1036; see Figure 2 (d), where LSQR finds its best regularized solution at iteration  $k^* = 24$ , much more early than the TSVD method, which computes the best regularized solution at  $k_0 = 9241$ , quite close to  $n$ . Based on Theorem 3.1, this indicates that the  $k$  Ritz values  $\theta_i^{(k)}$  must not approximate the large singular values of  $A$  in natural order for some  $k \leq k^*$ , and we will report numerical results in the next section. Nevertheless, the results illustrate that LSQR still has the full regularization.

This demonstrates that the approximations of the  $\theta_i^{(k)}$  to the large  $\sigma_i$  in natural order until the occurrence of semi-convergence of LSQR are *not necessary* conditions for the full regularization of LSQR. We have also used CGME and LSMR to solve this problem and found that LSMR has the full regularization too, but CGME computes a considerably less accurate regularized solution at its semi-convergence and thus has only the partial regularization; here we omit details on the numerical results obtained by CGME and LSMR.

In the following we test the 1D moderately ill-posed **heat** of  $n = 10240$  from [37], and illustrate the sharpness of the estimates for (4.1) when inserting (4.25) and (4.26) into it, where we again take the equalities in (4.25) and (4.26). Regarding the determination of  $\alpha$ , we compare the first 1000 singular values of **heat** with the model singular values  $\sigma_1/k^3$ , and we find that the model singular values first decay somewhat faster than those of **heat** and the rest ones decay more slowly than those of **heat**. As a result, we take  $\alpha = 3$  as a rough estimate, and use it in our estimates.

Figure 3 (a) plots the curves of  $|L_j^{(k)}(0)|$ ,  $j = 1, 2, \dots, k$  and  $k = 6, 7, \dots, 15$ . It is clear that  $|L_j^{(k)}(0)|$  increases with  $k$  for a given  $j$  and exhibits an apparent increasing tendency with  $j$  for a given  $k$ . Figure 3 (b) shows that, unlike for the severely ill-posed problem **shaw**,  $|L_{k_1}^{(k)}(0)|$  now increases substantially with  $k$  and  $\max_{k=2,3,\dots,35} |L_{k_1}^{(k)}(0)| \approx 1708$ , considerably bigger than one, but it increases much more slowly than it does for the mildly ill-posed problem **PRblurmotion**. Figure 3 (c) indicates that our estimates for  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  match the exact ones quite well for  $k = 1, 2, \dots, 35$ . We have found that the maximum and minimum of ratios of the estimated and true ones are 1.1911 and 0.8241, respectively, and the geometric mean of the ratios is 1.0167. All these results indicate that our estimates for  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  are sharp. We also plot the semi-convergence process of LSQR and the TSVD method; see Figure 3 (d), where the transition point  $k_0 = 35$  of the TSVD method but the semi-convergence of LSQR occurs at  $k^* = 26$ , considerably smaller than  $k_0$ . It follows from Theorem 3.1 that the  $k$  Ritz values  $\theta_i^{(k)}$  must not approximate the large singular values of  $A$  in natural order for some  $k \leq k^*$ . We will report numerical justifications in the next section. Remarkably, we see that the best LSQR solution  $x_{k^*}^{lsqr}$  is as accurate as the best TSVD solution  $x_{k_0}^{tsvd}$ . Again, this indicates that the approximations of the  $\theta_i^{(k)}$  to the large  $\sigma_i$  in natural order until the occurrence of semi-convergence of LSQR are *not necessary* conditions for the full regularization of LSQR. We have also tested CGME and LSMR, and found LSMR has the full regularization but CGME has only the partial regularization; the details are omitted here.

Finally, we pay special attention to  $|L_j^{(k)}(0)|$  and give more transparent numerical supports for Theorem 4.5 and Remark 4.4. Precisely, for  $k = 2, 3, \dots, 10$  we compute  $|L_j^{(k)}(0)|$  and their rough upper bounds  $1 + \frac{k}{2\alpha+1}$  when  $\alpha > 1$  for the model singular values  $\sigma_i = \frac{1}{i^\alpha}$  with  $\alpha = 0.6, 1, 3$  and 4. Together with Figure 3 (b) for **heat** and the observations on them, we have found that (i) the smaller  $\alpha$  is, the bigger  $|L_{k_1}^{(k)}(0)|$  is for the same  $k$  and (ii) the bigger  $\alpha$  is, the smaller  $|L_j^{(k)}(0)|$  is for a fixed  $k$  and the same small  $j$ . Moreover, we have found that, for  $k = 10$ ,  $|L_{k_1}^{(k)}(0)| \approx 3962.7$  for  $\alpha = 0.6$ ,  $|L_{k_1}^{(k)}(0)| \approx 199.88$  for  $\alpha = 1$ ,  $|L_{k_1}^{(k)}(0)| \approx 3.5103$  for  $\alpha = 3$ , and  $|L_{k_1}^{(k)}(0)| \approx 2.2877$  for  $\alpha = 4$ . Actually, the approximate upper bounds  $1 + \frac{k}{2\alpha+1}$  are 2.4286 and 2.1111 for  $\alpha = 3$  and 4, respectively. Therefore,  $1 + \frac{k}{2\alpha+1}$  is indeed a reasonably good estimate for  $|L_{k_1}^{(k)}(0)|$  for suitable  $\alpha > 1$ ; the bigger  $\alpha$ , the more accurate  $1 + \frac{k}{2\alpha+1}$  is as an estimate



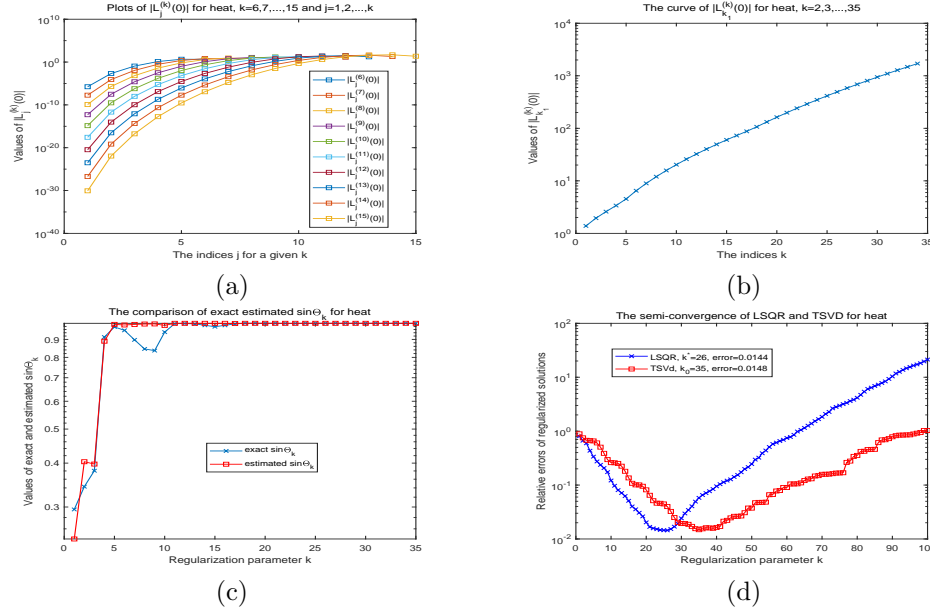


FIG. 3. (a): plots of  $|L_j^{(k)}(0)|$  for  $k = 6, 7, \dots, 15$ ; (b): the curve of  $|L_{k_1}^{(k)}(0)|$  for  $k = 2, 3, \dots, 35$ ; (c): the exact and estimated  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$ ; (d): the semi-convergence process of LSQR and TSVD.

for  $|L_{k_1}^{(k)}(0)|$ . On the other hand, if  $\alpha$  is small,  $1 + \frac{k}{2\alpha+1}$  underestimates  $|L_{k_1}^{(k)}(0)|$  very considerably. For  $k = 2, 3, \dots, 10$ , we have also observed that  $|L_{k_1}^{(k)}(0)| > \frac{k}{2\alpha+1}$  always holds, confirming the low bounds in (4.30) and (4.31).

**5. The effects of  $\sin \Theta$  theorem on the smallest Ritz value  $\theta_k^{(k)}$ .** In this section, we investigate how  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  affects the smallest Ritz value  $\theta_k^{(k)}$ . We aim at achieving a manifestation that (i) we *may* have  $\theta_k^{(k)} > \sigma_{k+1}$  for suitable  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| < 1$ , and (ii) we *must* have  $\theta_k^{(k)} < \sigma_{k+1}$ , that is, the  $k$  Ritz values  $\theta_i^{(k)}$  do not approximate the large singular values  $\sigma_i$  of  $A$  in natural order when  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  is sufficiently close to one. As it will turn out, the occurrence of (i) or (ii) has different requirements on the size of  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  for the three kinds of ill-posed problems.

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

$$(5.1) \quad \varepsilon_k^2 \sigma_k^2 + (1 - \varepsilon_k^2) \sigma_n^2 < \tilde{q}_k^T A^T A \tilde{q}_k < \varepsilon_k^2 \sigma_{k+1}^2 + (1 - \varepsilon_k^2) \sigma_1^2.$$

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

$$(5.2) \quad \sqrt{\tilde{q}_k^T A^T A \tilde{q}_k} > \sigma_{k+1};$$

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

$$(5.3) \quad \theta_k^{(k)} < (1 + \delta)^{1/2} \sigma_{k+1},$$

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

*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

$$\begin{aligned} \|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| &= \|(V_k^\perp)^T Q_k\| = \|V_k^\perp (V_k^\perp)^T Q_k\| \\ &= \max_{\|c\|=1} \|V_k^\perp (V_k^\perp)^T Q_k c\| = \|V_k^\perp (V_k^\perp)^T Q_k c_k\| \\ (5.4) \quad &= \|V_k^\perp (V_k^\perp)^T \tilde{q}_k\| = \|(V_k^\perp)^T \tilde{q}_k\| = \sqrt{1 - \varepsilon_k^2} \end{aligned}$$

with  $\tilde{q}_k = Q_k c_k \in \mathcal{V}_k^R$  and  $\|c_k\| = 1$ .

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

$$(5.5) \quad \tilde{q}_k = V_k^\perp (V_k^\perp)^T \tilde{q}_k + V_k V_k^T \tilde{q}_k.$$

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

$$(5.6) \quad \|V_k^T \tilde{q}_k\| = \|V_k V_k^T \tilde{q}_k\| = \sqrt{1 - \|V_k^\perp (V_k^\perp)^T \tilde{q}_k\|^2} = \sqrt{1 - (1 - \varepsilon_k^2)} = \varepsilon_k.$$

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

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

where  $\Sigma_k = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_k)$  and  $\Sigma_k^\perp = \text{diag}(\sigma_{k+1}, \sigma_{k+2}, \dots, \sigma_n)$ . 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

$$\begin{aligned} \tilde{q}_k^T A^T A \tilde{q}_k &= (V_k^\perp (V_k^\perp)^T \tilde{q}_k + V_k V_k^T \tilde{q}_k)^T A^T A (V_k^\perp (V_k^\perp)^T \tilde{q}_k + V_k V_k^T \tilde{q}_k) \\ &= (\tilde{q}_k^T V_k^\perp (V_k^\perp)^T + \tilde{q}_k^T V_k V_k^T) (V_k^\perp (\Sigma_k^\perp)^2 (V_k^\perp)^T \tilde{q}_k + V_k \Sigma_k^2 V_k^T \tilde{q}_k) \\ (5.7) \quad &= \tilde{q}_k^T V_k^\perp (\Sigma_k^\perp)^2 (V_k^\perp)^T \tilde{q}_k + \tilde{q}_k^T V_k \Sigma_k^2 V_k^T \tilde{q}_k. \end{aligned}$$

$(V_k^\perp)^T \tilde{q}_k$  and  $V_k^T \tilde{q}_k$  are unlikely 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  $e_{n-k}^{(n-k)}$  of  $\mathbb{R}^{n-k}$  and the  $k$ -th canonical vector  $e_k^{(k)}$  of  $\mathbb{R}^k$ , respectively; otherwise,  $\tilde{q}_k = v_n$  and  $\tilde{q}_k = v_k$  simultaneously, which are impossible as  $k < n$ . Therefore, from (5.7), (5.4) and (5.6), we obtain the strict inequality

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

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

$$\tilde{q}_k^T A^T A \tilde{q}_k < \|(V_k^\perp)^T \tilde{q}_k\|^2 \|(\Sigma_k^\perp)^2\| + \|V_k^T \tilde{q}_k\|^2 \|\Sigma_k^2\| = (1 - \varepsilon_k^2) \sigma_{k+1}^2 + \varepsilon_k^2 \sigma_1^2.$$

From the lower bound of (5.1), we see that if  $\varepsilon_k$  satisfies  $\varepsilon_k^2 \sigma_k^2 \geq \sigma_{k+1}^2$ , i.e.,  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$ , then  $\sqrt{\tilde{q}_k^T A^T A \tilde{q}_k} > \sigma_{k+1}$ , i.e., (5.2) holds.

From (2.4), 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

$$(5.8) \quad (\theta_k^{(k)})^2 = \min_{\|c\|=1} c^T Q_k^T A^T A Q_k c = \min_{q \in \mathcal{V}_k^R, \|q\|=1} q^T A^T A q = \hat{q}_k^T A^T A \hat{q}_k,$$

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

$$(5.9) \quad \theta_k^{(k)} \leq \sqrt{\tilde{q}_k^T A^T A \tilde{q}_k},$$

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

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

i.e., (5.3) holds, solving which for  $\varepsilon_k^2$  gives  $\varepsilon_k^2 \leq \frac{\delta}{(\frac{\sigma_1}{\sigma_{k+1}})^2 - 1}$ .  $\square$

In the sense of (5.8),  $\hat{q}_k \in \mathcal{V}_k^R$  is the optimal vector that extracts the least information from  $\mathcal{V}_k$  and the richest information from  $\text{span}\{V_k^\perp\}$ . From the assumption on  $\tilde{q}_k$ , since  $\mathcal{V}_k$  is the orthogonal complement of  $\text{span}\{V_k^\perp\}$ , 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  $\text{span}\{V_k^\perp\}$ . Therefore,  $\hat{q}_k$  and  $\tilde{q}_k$  have a similar optimality, and consequently

$$(5.10) \quad \theta_k^{(k)} \approx \sqrt{\tilde{q}_k^T A^T A \tilde{q}_k}.$$

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

We analyze  $\theta_k^{(k)}$  and inspect the condition  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$  for (5.2). It is known that  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k} \sim \rho^{-1}$  for severely ill-posed problems, meaning that  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  is approximately smaller than  $1 - \frac{1}{2}\rho^{-2}$ . For moderately ill-posed problems, the lower bound  $\sigma_{k+1}/\sigma_k$  increases with  $k$ , and it cannot be close to one for suitable  $\alpha > 1$ ; for mildly ill-posed problems, the lower bound for  $\varepsilon_k$  increases faster than it does for moderately ill-posed problems since  $\alpha \leq 1$ , and, furthermore, it may well approach one for  $k$  small. In conclusion, the condition  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$  for (5.2) requires that  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  be not close to one for severely and moderately ill-posed problems with suitable  $\alpha > 1$ , but it must be fairly small for mildly ill-posed problems.

We now investigate if the true, i.e., actual  $\varepsilon_k$  resulting from the three kinds of ill-posed problems satisfies the condition  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$  for (5.2). In view of (4.1) 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  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$  for (5.2) amounts to requiring that  $\|\Delta_k\|$  cannot be large for severely and moderately ill-posed problems but it must be fairly small for mildly ill-posed problems. Unfortunately, Theorems 4.2–4.4 and the remarks on them indicate that  $\|\Delta_k\|$  is approximately  $\rho^{-(2+\beta)}$  by (4.22) and (4.23) for  $k \leq k_0$ , considerably smaller than one for a severely ill-posed problem with  $\rho > 1$  not close to one, it is modest and increases slowly with  $k$  for a moderately ill-posed problem with suitable  $\alpha > 1$ , and it increases with  $k$  and is generally large for a mildly ill-posed problem. Consequently, for mildly ill-posed problems, the actual  $\|\Delta_k\|$  can hardly be small and is generally large, namely, the true  $\varepsilon_k$  is small, which causes that the condition  $\varepsilon_k \geq \frac{\sigma_{k+1}}{\sigma_k}$  fails to meet soon as  $k$  increases, while it is satisfied for severely or moderately ill-posed problems with suitable  $\rho > 1$  or  $\alpha > 1$  for  $k$  small.

We report numerical experiments to confirm Theorem 5.1 and the above remarks. Besides the previous severely, moderately and mildly problems `shaw`, `heat`, `PRblurmotion`, we also test the 1D moderately ill-posed problem `deriv2` of  $n = 10000$  [37] and

the 2D mildly ill-posed problems PRspherical of  $m = 14100, n = 10000$  and PRseismic of  $m = 20000, n = 10000$ , which are from seismic travel-time tomography and spherical means tomography [21], respectively. For the latter three problems, except the matrix orders, we take all the other parameter(s) as default(s). The singular values  $\sigma_k$  of deriv2 decay exactly like  $\frac{1}{k^2}$  (cf. [39, p.21]); the singular values of PRspherical and PRseismic decay roughly like  $\sigma_1/k^{0.6}$  in an initial stage, we add Gaussian white noises with the relative level  $\varepsilon = 0.05$  to the right-hand sides  $b_{true}$  of PRspherical and PRseismic, respectively. The noise level  $\varepsilon = 0.001$  is used in shaw, heat and deriv2, and  $\varepsilon = 0.01$  is used in PRblurmotion, the same as that in the last section.

For each of the six problems, we first investigate the true  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  and the required sufficient conditions  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| = \sqrt{1 - \varepsilon_k^2}$  that makes (5.2) hold, from which, (5.9) and (5.10) it is known that  $\theta_k^{(k)} > \sigma_{k+1}$  may hold. In the tests, we take  $\varepsilon_k = \frac{\sigma_{k+1}}{\sigma_k}$  and compute  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\| = \sqrt{1 - \varepsilon_k^2}$ . We check how the required sufficient conditions are met for each problem and a given  $k$ . We depict the true  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  versus the required ones in Figures 4–9 (a) and draw the comparison diagrams of  $k$  Ritz values  $\theta_i^{(k)}$  and first  $k + 1$  large singular values  $\sigma_i$  for each  $k$  in Figures 4–9 (b).

Figure 4 (a) indicates that for shaw the required sufficient conditions are fulfilled in the first 20 iterations except for  $k = 18$ . Figures 5 (a) and Figures 7–9 (a) show that for heat, deriv2, PRspherical and PRseismic the sufficient conditions on  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  are satisfied until  $k = 3, k = 5, k = 2$  and  $k = 1$ , respectively, after which the true  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  starts to increase and approaches one quickly; for PRblurmotion, it is even worse that the required  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  are never met for any  $k \geq 1$ , as shown by Figure 6 (a). These results justify our theory that (i) the required  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  are met more easily for severely ill-posed problems than for moderately and mildly ill-posed problems; (ii) the required  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  are fairly small for moderately and especially mildly ill-posed problems, but the true  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  approach one as  $k$  increases and they tend to one faster for mildly ill-posed problems; (iii) for moderately and mildly ill-posed problems the true  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  exhibit monotonically increasing tendency and approach one with  $k$ , which confirms our results.

Next we numerically investigate the behavior of the smallest Ritz value  $\theta_k^{(k)}$  and verify close relationships between it and the required sufficient condition on  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  that ensures  $\theta_k^{(k)} > \sigma_{k+1}$ . For shaw, we see from Figure 4 (b) that all the  $\theta_k^{(k)}$  are above  $\sigma_{k+1}$  for  $k = 1, 2, \dots, 20$ , including  $k = 18$  at which the sufficient condition fails to meet. This indicates that the sufficient condition is not necessary for ensuring  $\theta_k^{(k)} > \sigma_{k+1}$ . For heat, Figure 5 (b) clearly shows that the  $k$  Ritz values  $\theta_i^{(k)}$  approximate the first  $k$  large singular values  $\sigma_i$  of heat, which includes  $\theta_k^{(k)} > \sigma_{k+1}$ , for  $k = 1, 2, 3$ , at which the required sufficient conditions are satisfied, and  $\theta_k^{(k)} < \sigma_{k+1}$  appears exactly from  $k = 4$  onwards. This example illustrates that the required sufficient condition is also necessary, for if they are not met then  $\theta_k^{(k)} < \sigma_{k+1}$ . The numerical results on deriv2 are similar to those on heat; from Figure 7 (b), we see that  $\theta_k^{(k)} > \sigma_{k+1}$  until  $k = 6$ , after which the required sufficient condition fails to fulfill and  $\theta_k^{(k)} < \sigma_{k+1}$  occurs.

For the mildly ill-posed PRblurmotion, notice that the required sufficient conditions on  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  fail to meet for all  $k \geq 1$ . By Theorem 5.1, the  $k$  Ritz values  $\theta_i^{(k)}$  may not approximate the first  $k$  singular values  $\sigma_i$  in natural order for all  $k \geq 1$ . This is indeed the case, as shown clearly by Figure 6 (b), which shows that all the

$\theta_k^{(k)}$  are below  $\sigma_{k+1}$ . Regarding the mildly ill-posed PRspherical and PRseismic, the sufficient conditions are satisfied only for  $k = 1$ , as is seen from Figures 8–9 (a). The  $k$  Ritz values  $\theta_i^{(k)}$  interlace the first  $k + 1$  large singular values  $\sigma_i$  in natural order only for  $k = 1$ , and afterwards  $\theta_k^{(k)} < \sigma_{k+1}$ , as indicated clearly by Figures 8–9 (b). For these two problems, at iteration  $k = 1$  the Ritz value  $\theta_1^{(1)}$  lies between  $\sigma_1$  and  $\sigma_2$  and is closer to  $\sigma_1$ . Again, these results demonstrate that our sufficient conditions are tight. Moreover, compared with the previous problems, we find that, generally, the more slowly the singular values  $\sigma_i$  decay, the harder the sufficient condition is to fulfill, and the sooner  $\theta_k^{(k)} < \sigma_{k+1}$  occurs.

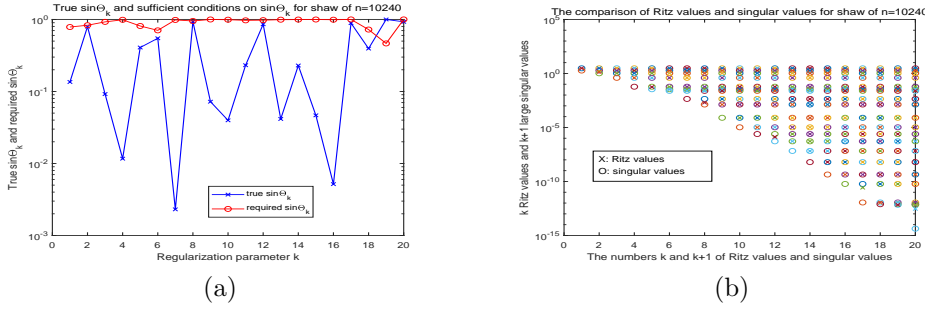


FIG. 4. (a): The true  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  and the required sufficient conditions on them; (b):  $k$  Ritz values and the first  $k + 1$  large singular values of shaw,  $k = 1, 2, \dots, 20$ .

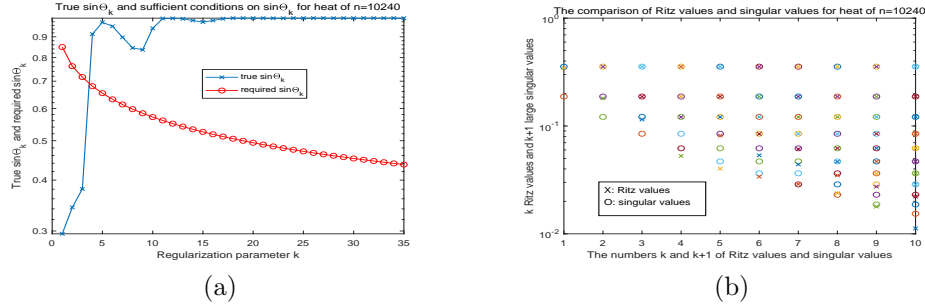


FIG. 5. (a) The true  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  and the required sufficient conditions on them; (b):  $k$  Ritz values and the first  $k + 1$  large singular values of heat,  $k = 1, 2, \dots, 10$ .

In Figure 10, we depict the semi-convergence processes of LSQR and the TSVD method for PRseismic, where it is seen that  $k^* = 8$  and  $k_0 = 1669$ . In Figure 11, we depict the semi-convergence processes of LSQR and the TSVD method for deriv2 and PRspherical, where the semi-convergence point  $k^* = 21$  of LSQR and the transition point  $k_0 = 47$  of the TSVD method for deriv2, and  $k^* = 12$  and  $k_0 = 6006$  for PRspherical. For these three problems, we find that  $k^* \ll k_0$ , especially for PRseismic and PRspherical. However, it is clear from the figures that the best regularized solutions by LSQR are at least as accurate as those computed by the TSVD method. Again, they results illustrate that the approximations of  $\theta_i^{(k)}$  to the large  $\sigma_i$  in natural order until the occurrence of semi-convergence of LSQR are *not necessary* conditions for the full regularization of LSQR.

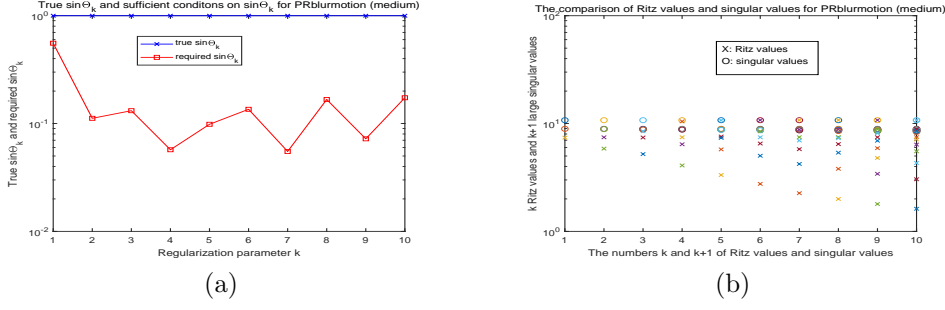


FIG. 6. (a): The true  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  and the required sufficient conditions on them; (b):  $k$  Ritz values and the first  $k+1$  large singular values of PRblurmotion,  $k = 1, 2, \dots, 10$ .

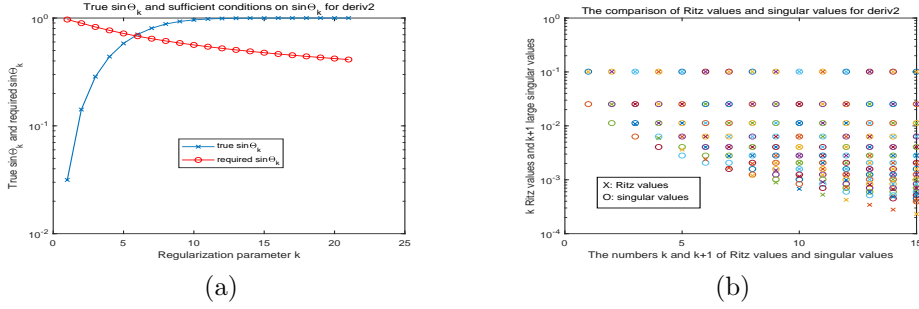


FIG. 7. (a): The true  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  and the required sufficient conditions on them; (b):  $k$  Ritz values and the first  $k+1$  large singular values of deriv2,  $k = 1, 2, \dots, 15$ .

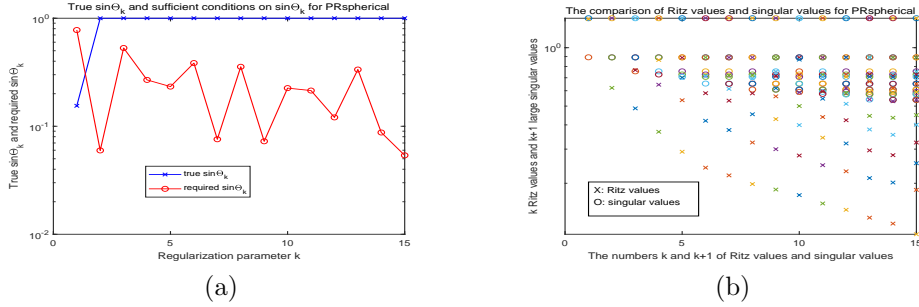


FIG. 8. (a): The true  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  and the required sufficient conditions on them; (b):  $k$  Ritz values and the first  $k+1$  large singular values of PRspherical,  $k = 1, 2, \dots, 10$ .

**6. Conclusions.** For a general large-scale linear discrete ill-posed problem (1.1), the Krylov iterative solvers LSQR and CGLS are most popularly used, and they, together with CGME and LSMR, are deterministic 2-norm filtering iterative regularization methods. These methods have general regularizing effects and exhibit semi-convergence. For each of them, if the regularized solution at semi-convergence are as accurate as the best one obtained by the TSVD method, which has been known to find a 2-norm filtering best possible solution, the method has the full regularization. In this case, for a given problem, once the semi-convergence is practically recognized, we have computed a best possible regularized solution and simply stop the method. The determination of semi-convergence can, in principle, be determined by a suitable

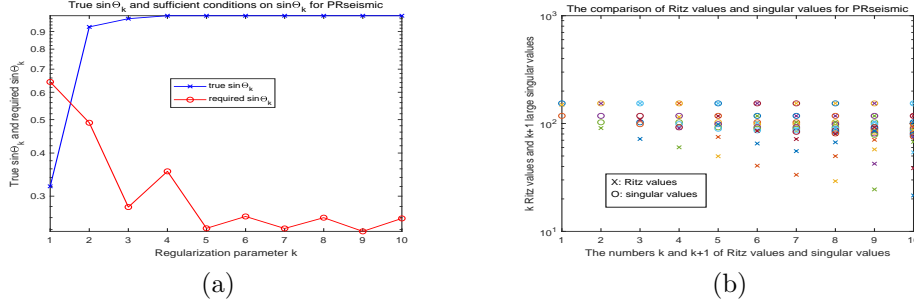


FIG. 9. (a): The true  $\|\sin \Theta(\mathcal{V}_k, \mathcal{V}_k^R)\|$  and the required sufficient conditions on them; (b):  $k$  Ritz values and the first  $k+1$  large singular values of PRseismic,  $k = 1, 2, \dots, 10$ .

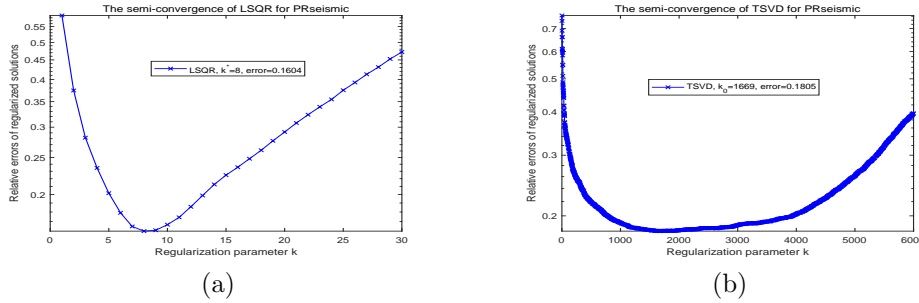


FIG. 10. (a)-(b): The semi-convergence processes of LSQR and TSVD for PRseismic.

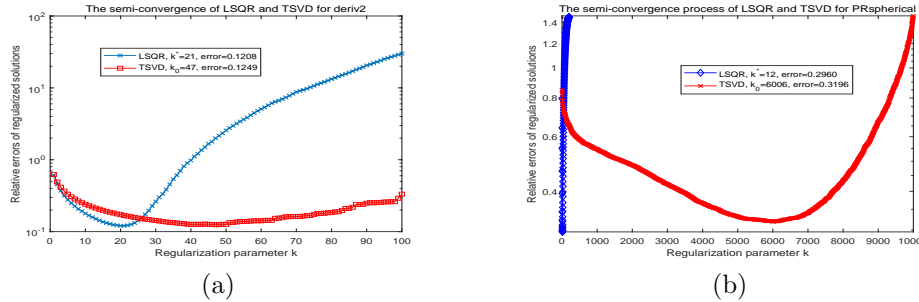


FIG. 11. (a): the semi-convergence process of LSQR and TSVD for deriv2; (b): the semi-convergence process of LSQR and TSVD for PRspherical2.

parameter-choice method, such as the L-curve criterion and the discrepancy principle.

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



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

Very surprisingly, we have found that for all the test problems, independent of the degree of ill-posedness of (1.1), the LSQR best regularized solutions  $x_{k^*}^{lsqr}$  are as accurate as the TSVD best solutions  $x_{k_0}^{tsvd}$ . This indicates that LSQR has the full regularization for the test problems, even though the Ritz values do not approximate the large singular values of  $A$  in natural before some  $k \leq k^*$ . We have made numerical experiments on each of the test problems for different noise levels  $\varepsilon$  and have had the same findings. Furthermore, we have observed that LSMR has the full regularization too for the test problems, but it is not the case for CGME, whose best regularized solutions are considerably less accurate than and can hardly be as accurate as those by LSQR, even for severely ill-posed problems. Therefore, the full or partial regularization of these Krylov solvers is much more complicated than one may have expected, and deserves high attention and in-depth study.

#### REFERENCES

- [1] R. C. Aster, B. Borchers, and C. H. Thurber, *Parameter Estimation and Inverse Problems*, second ed., Elsevier, New York, 2013.
- [2] Z. Bai, J. Demmel, J. Dongarra, A. Ruhe, and H. A. van der Vorst, *Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide*, vol. 11, SIAM, Philadelphia, PA, 2000.
- [3] F. Bauer and M. A. Lukas, *Comparing parameter choice methods for regularization of ill-posed problems*, Math. Comput. Simul., 81 (2011), pp. 1795–1841.
- [4] F. S. V. Bazán and L. S. Borges, *GKB-FP: an algorithm for large-scale discrete ill-posed problems*, BIT Numer. Math., 50 (2010), pp. 481–507.
- [5] F. S. V. Bazán, M. C. C. Cunha, and L. S. Borges, *Extension of GKB-FP algorithm to large-scale general-form Tikhonov regularization*, Numer. Linear Algebra Appl., 21 (2014), pp. 316–339.
- [6] S. Berisha and J. G. Nagy, *Restore tools: Iterative methods for image restoration*, 2012, available from <http://www.mathcs.emory.edu/~nagy/RestoreTools>.
- [7] Å. Björck, *A bidiagonalization algorithm for solving large and sparse ill-posed systems of linear equations*, BIT, 28 (1988), pp. 659–670.
- [8] ———, *Numerical Methods for Least Squares Problems*, SIAM, Philadelphia, PA, 1996.
- [9] ———, *Numerical Methods in Matrix Computations*, Texts in Applied Mathematics, vol. 59, Springer, Cham, 2015.
- [10] Å. Björck and L. Eldén, *Methods in numerical algebra for ill-posed problems*, Report LiTH-R-33-1979, Dept. of Mathematics, Linköping University, Sweden, 1979.
- [11] Å. Björck, E. Grimme, and P. van Dooren, *An implicit shift bidiagonalization algorithm for ill-posed systems*, BIT Numer. Math., 34 (1994), pp. 510–534.
- [12] J. Chung, J. G. Nagy, and D. P. O’Leary, *A weighted-GCV method for Lanczos-hybrid regularization*, Electr. Trans. Numer. Anal., 28 (2007/08), pp. 149–167.
- [13] J. Chung and K. Palmer, *A hybrid LSMR algorithm for large-scale Tikhonov regularization*, SIAM J. Sci. Comput., 37 (2015), pp. S562–S580.
- [14] E. J. Craig, *The  $N$ -step iteration procedures*, J. Math. Phys. 34 (1955), pp. 64–73.
- [15] B. Eicke, A. K. Liou, and R. Plato, *The instability of some gradient methods for ill-posed problems*, Numer. Math., 58 (1990), pp. 129–134.
- [16] H. W. Engl, *Regularization methods for the stable solution of inverse problems*, Surveys Math. Indust., 3 (1993), pp. 71–143.
- [17] H. W. Engl, M. Hanke, and A. Neubauer, *Regularization of Inverse Problems*, Kluwer Academic Publishers, 2000.
- [18] R. D. Fierro, G. H. Golub, P. C. Hansen, and D. P. O’Leary, *Regularization by truncated total least squares*, SIAM J. Sci. Comput., 18 (1997), pp. 1223–1241.
- [19] D. C. L. Fong and M. Saunders, *LSMR: an iterative algorithm for sparse least-squares problems*, SIAM J. Sci. Comput., 33 (2011), pp. 2950–2971.

- [20] A. Frommer and P. Maass, *Fast CG-based methods for Tikhonov-Phillips regularization*, SIAM J. Sci. Comput., 20 (1999) pp. 1831–1850.
- [21] S. Gazzola, P. C. Hansen, and J. G. Nagy, *IR tools: A MATLAB package of iterative regularization methods and large-scale test problems*, Numer. Algor., doi.org/10.1007/s11075-018-0570-7.
- [22] S. Gazzola and P. Novati, *Inheritance of the discrete Picard condition in Krylov subspace methods*, BIT Numer. Math., 56 (2016), pp. 893–918.
- [23] S. Gazzola, P. Novati, and M. R. Russo, *On Krylov projection methods and Tikhonov regularization*, Electr. Trans. Numer. Anal., 44 (2015), pp. 83–123.
- [24] H. Gferefer, *An a posteriori parameter choice for ordinary and iterated tikhonov regularization of ill-posed problems leading to optimal convergence rates*, Math. Comput., 49 (1987), pp. 507–522.
- [25] S. F. Gilyazov, *Regularizing algorithms based on the conjugate gradient method*, U.S.S.R. Comput. Maths. Math. Phys., 26 (1986), pp. 8–13.
- [26] S. F. Gilyazov and N. L. Gol'dman, *Regularization of Ill-Posed Problems by Iteration Methods*, Mathematics and its Applications, vol. 499, Kluwer Academic Publishers, Dordrecht, 2000.
- [27] G. H. Golub, M. T. Heath, and G. Wahba, *Generalized cross-validation as a method for choosing a good ridge parameter*, Technometrics, 21 (1979), pp. 215–223.
- [28] G. H. Golub and D. P. O'Leary, *Some history of the conjugate gradient and Lanczos algorithms: 1948–1976*, SIAM Rev., 31 (1989), pp. 50–102.
- [29] M. Hanke, *Conjugate gradient Type Methods for Ill-Posed Problems*, Pitman Research Notes in Mathematics Series, vol. 327, Longman, Essex, 1995.
- [30] ———, *Limitations of the L-curve method in ill-posed problems*, BIT, 36 (1996), pp. 287–301.
- [31] ———, *On Lanczos based methods for the regularization of discrete ill-posed problems*, BIT Numer. Math., 41 (2001), Suppl., pp. 1008–1018.
- [32] M. Hanke and P. C. Hansen, *Regularization methods for large-scale problems*, Surveys Math. Indust., 3 (1993), pp. 253–315.
- [33] P. C. Hansen, *The discrete Picard condition for discrete ill-posed problems*, BIT, 30 (1990), pp. 658–672.
- [34] ———, *Truncated singular value decomposition solutions to discrete ill-posed problems with ill-determined numerical rank*, SIAM J. Sci. Statist. Comput., 11 (1990), pp. 503–518.
- [35] ———, *Analysis of discrete ill-posed problems by means of the L-curve*, SIAM Rev., 34 (1992), pp. 561–580.
- [36] ———, *Rank-Deficient and Discrete Ill-Posed Problems: Numerical Aspects of Linear Inversion*, SIAM Monographs on Mathematical Modeling and Computation, SIAM, Philadelphia, PA, 1998.
- [37] ———, *Regularization Tools version 4.0 for Matlab 7.3*, Numer. Algor., 46 (2007), pp. 189–194.
- [38] ———, *Regularization tools: A matlab package for analysis and solution of discrete ill-posed problems version 4.1 for matlab 7.3*, 2008, available from [www.netlib.org/numeralgo](http://www.netlib.org/numeralgo).
- [39] ———, *Discrete Inverse Problems: Insight and Algorithms*, Fundamentals of Algorithms, vol. 7, SIAM, Philadelphia, PA, 2010.
- [40] P. C. Hansen and D. P. O'Leary, *The use of the l-curve in the regularization of discrete ill-posed problems*, SIAM J. Sci. Comput., 14 (1993), pp. 1487–1503.
- [41] P. C. Hansen, V. Pereyra, and G. Scherer, *Least Squares Data Fitting with Applications*, The Johns Hopkins University Press, Baltimore, MD, 2013.
- [42] M. R. Hestenes and E. Stiefel, *Methods of conjugate gradients for solving linear systems*, J. Res. Nat. Bur. Stand., 49 (1952), pp. 409–436.
- [43] M. R. Hnětynková, Marie Kubínová, and M. Plešinger, *Noise representation in residuals of LSQR, LSMR, and Craig regularization*, Linear Algebra Appl., 533 (2017), pp. 357–379.
- [44] M. R. Hnětynková, M. Plešinger, and Z. Strakoš, *The regularizing effect of the Golub-Kahan iterative bidiagonalization and revealing the noise level in the data*, BIT Numer. Math., 49 (2009), pp. 669–696.
- [45] B. Hofmann, *Regularization for Applied Inverse and Ill-Posed Problems*, Teubner, Stuttgart, Germany, 1986.
- [46] Y. Huang and Z. Jia, *Some results on the regularization of LSQR for large-scale ill-posed problems*, Science China Math., 60 (2017), pp. 701–718.
- [47] K. Ito and B. Jin, *Inverse Problems: Tikhonov Theory and Algorithms*, Series on Applied Mathematics, vol. 22, World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2015.
- [48] Z. Jia, *The convergence of harmonic Ritz values, harmonic Ritz vectors, and refined harmonic Ritz vectors*, Math. Comput., 74 (2005), pp. 1441–1456.
- [49] Z. Jia and D. Niu, *An implicitly restarted refined bidiagonalization Lanczos method for computing a partial singular value decomposition*, SIAM J. Matrix Anal. Appl., 25 (2003),

- pp. 246–265.
- [50] ———, *A refined harmonic Lanczos bidiagonalization method and an implicitly restarted algorithm for computing the smallest singular triplets of large matrices*, SIAM J. Sci. Comput., 32 (2010), pp. 714–744.
  - [51] C. Johnsson, *On finite element methods for optimal control problems*, Tech. Report 79-04 R, Dept. of Computer Science, University of Gothenburg, 1979.
  - [52] J. Kaipio and E. Somersalo, *Statistical and Computational Inverse Problems*, Applied Mathematical Sciences, vol. 160, Springer-Verlag, New York, 2005.
  - [53] M. Kern, *Numerical Methods for Inverse Problems*, John Wiley & Sons, Inc., 2016.
  - [54] M. E. Kilmer and D. P. O’Leary, *Choosing regularization parameters in iterative methods for ill-posed problems*, SIAM J. Matrix Anal. Appl., 22 (2001), pp. 1204–1221.
  - [55] S. Kindermann, *Convergence analysis of minimization-based noise level-free parameter choice rules for linear ill-posed problems*, Electr. Trans. Numer. Anal., 38 (2011), pp. 233–257.
  - [56] A. Kirsch, *An Introduction to the Mathematical Theory of Inverse problems*, second ed., Applied Mathematical Sciences, vol. 120, Springer, New York, 2011.
  - [57] P. K. Kytte and P. Puri, *Computational Methods for Linear Integral Equations*, Birkhäuser Boston, Inc., Boston, MA, 2002.
  - [58] R. A. Lawson and R. J. Hanson, *Solving Least Squares Problems*, Classics in Applied Mathematics, vol. 15, SIAM, Philadelphia, PA, 1995, Revised reprint of the 1974 original edition.
  - [59] B. Lewis and L. Reichel, *Arnoldi-Tikhonov regularization methods*, J. Comput. Appl. Math., 226 (2009), pp. 92–102.
  - [60] K. Miller, *Least squares methods for ill-posed problems with a prescribed bound.*, SIAM J. Math. Anal., 1 (1970), pp. 52–74.
  - [61] V. A. Morozov, *On the solution of functional equations by the method of regularization*, Soviet Math. Dokl., 7 (1966), pp. 414–417.
  - [62] J. L. Mueller and S. Siltanen, *Linear and Nonlinear Inverse Problems with Practical Applications*, Computational Science & Engineering, vol. 10, SIAM, Philadelphia, PA, 2012.
  - [63] F. Natterer, *The Mathematics of Computerized Tomography*, Classics in Applied Mathematics, vol. 32, SIAM, Philadelphia, PA, 2001, Reprint of the 1986 original edition.
  - [64] A. S. Nemirovskii, *The regularizing properties of the adjoint gradient method in ill-posed problems*, U.S.S.R. Comput. Maths. Math. Phys., 26 (1986), pp. 7–16.
  - [65] A. Neumaier, *Solving ill-conditioned and singular linear systems: a tutorial on regularization*, SIAM Rev., 40 (1998), pp. 636–666.
  - [66] A. Neuman, L. Reichel, and H. Sadok, *Algorithms for range restricted iterative methods for linear discrete ill-posed problems*, Numer. Algor., 59 (2012), pp. 325–331.
  - [67] G. Nolet, *Solving or resolving inadequate and noisy tomographic systems*, J. Comput. Phys., 61 (1985), pp. 463–482.
  - [68] D. P. O’Leary and J. A. Simmons, *A bidiagonalization-regularization procedure for large scale discretizations of ill-posed problems*, SIAM J. Sci. Statist. Comput., 2 (1981), pp. 474–489.
  - [69] C. C. Paige and M. A. Saunders, *Solutions of sparse indefinite systems of linear equations*, SIAM J. Numer. Anal., 12 (1975), pp. 617–629.
  - [70] ———, *LSQR: an algorithm for sparse linear equations and sparse least squares*, ACM Trans. Math. Software, 8 (1982), pp. 43–71.
  - [71] C. C. Paige and Z. Z. Strakoš, *Core problems in linear algebraic systems*, SIAM J. Matrix Anal. Appl., 27 (2005), pp. 861–875.
  - [72] B. N. Parlett, *The Symmetric Eigenvalue Problem*, Classics in Applied Mathematics, vol. 20, SIAM, Philadelphia, PA, 1998, Corrected reprint of the 1980 original.
  - [73] D. L. Phillips, *A technique for the numerical solution of certain integral equations of the first kind*, J. Assoc. Comput. Mach. 9 (1962), 84–97.
  - [74] T. Raus, *The principle of the residual in the solution of ill-posed problems with nonselfadjoint operator*, Uchen. Zap. Tartu Gos. Univ., 75 (1985), pp. 12–20.
  - [75] R. A. Renaut, S. Vatankehah, and V. E. Ardestani, *Hybrid and iteratively reweighted regularization by unbiased predictive risk and weighted GCV*, SIAM J. Sci. Comput., 39 (2017), pp. B221–B243.
  - [76] J. A. Scales and A. Gerztenkorn, *Robust methods in inverse theory*, Inverse Probl., 4 (1988), pp. 1071–1091.
  - [77] W. Squire, *The solution of ill-conditioned linear systems arising from Fredholm equations of the first kind by steepest descents and conjugate gradients*, Internat. J. Numer. Methods Engrg., 10 (1976), pp. 607–617.
  - [78] G. W. Stewart, *Matrix Algorithms I: Basic Decompositions*, SIAM, Philadelphia, PA, 1998.
  - [79] ———, *Matrix Algorithms II: Eigensystems*, SIAM, Philadelphia, PA, 2001.
  - [80] G. W. Stewart and J.-G. Sun, *Matrix Perturbation Theory*, Computer Science and Scientific

- Computing, Academic Press, Inc., Boston, MA, 1990.
- [81] A. A. Tal, *Numerical solution of Fredholm integral equations of the first kind*, TR-66-34, Computer Science Center, University of Maryland, College Park, MD, 1966.
  - [82] A. N. Tikhonov, *On the solution of ill-posed problems and the method of regularization*, Dokl. Akad. Nauk SSSR, 151 (1963), pp. 501–504.
  - [83] A. N. Tikhonov and V. Y. Arsenin, *Solutions of Ill-Posed Problems*, V. H. Winston & Sons, Washington, D.C., 1977.
  - [84] A. van der Sluis and H. A. van der Vorst, *The rate of convergence of conjugate gradients*, Numer. Math., 48 (1986), pp. 543–560.
  - [85] ———, *SIRT- and CG-type methods for the iterative solution of sparse linear least-squares problems*, Linear Algebra Appl., 130 (1990), pp. 257–303.
  - [86] H. A. van der Vorst, *Computational Methods for Large Eigenvalue Problems*, Handbook of Numerical Analysis, Vol. VIII, North-Holland, Amsterdam, 2002, pp. 3–179.
  - [87] J. M. Varah, *On the numerical solution of ill-conditioned linear systems with applications to ill-posed problems*, SIAM J. Numer. Anal., 10 (1973), pp. 257–267.
  - [88] ———, *A practical examination of some numerical methods for linear discrete ill-posed problems*, SIAM Rev., 21 (1979), pp. 100–111.
  - [89] C. R. Vogel, *Non-convergence of the L-curve regularization parameter selection method*, Inverse Probl., 12 (1996), pp. 535–547.
  - [90] ———, *Computational Methods for Inverse Problems*, Frontiers in Applied Mathematics, vol. 23, SIAM, Philadelphia, PA, 2002.
  - [91] G. Wahba, *Practical approximate solutions to linear operator equations when the data are noisy*, SIAM J. Numer. Anal., 14 (1977), pp. 651–667.