A REFINED HARMONIC LANCZOS BIDIAGONALIZATION
METHOD AND AN IMPLICITLY RESTARTED ALGORITHM FOR
COMPUTING THE SMALLEST SINGULAR TRIPLETS OF LARGE
MATRICES
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Abstract. The harmonic Lanczos bidiagonalization method can be used to compute the smallest singular triplets of a large matrix $A$. We prove that for good enough projection subspaces harmonic Ritz values converge if the columns of $A$ are strongly linearly independent. On the other hand, harmonic Ritz values may miss some desired singular values when the columns of $A$ are almost linearly dependent. Furthermore, harmonic Ritz vectors may converge irregularly and even may fail to converge. Based on the refined projection principle for large matrix eigenproblems due to the first author, we propose a refined harmonic Lanczos bidiagonalization method that takes the Rayleigh quotients of the harmonic Ritz vectors as approximate singular values and extracts the best approximate singular vectors, called the refined harmonic Ritz approximations, from the given subspaces in the sense of residual minimizations. The refined approximations are shown to converge to the desired singular vectors once the subspaces are sufficiently good and the Rayleigh quotients converge. An implicitly restarted refined harmonic Lanczos bidiagonalization algorithm (IRRHLB) is developed. We study how to select the best possible shifts, and suggest refined harmonic shifts that are theoretically better than the harmonic shifts used within the implicitly restarted Lanczos bidiagonalization algorithm (IRHLB). We propose a novel procedure that can numerically compute the refined harmonic shifts efficiently and accurately. Numerical experiments are reported that compare IRRHLB with five other algorithms based on the Lanczos bidiagonalization process. It appears that IRRHLB is at least competitive with them and can be considerably more efficient when computing the smallest singular triplets.

Key words. singular values, singular vectors, SVD, Lanczos bidiagonalization, refined projection, harmonic, refined harmonic, implicit restart, harmonic shifts, refined harmonic shifts.

AMS subject classifications. 65F15, 15A18

1. Introduction. We assume that a large sparse matrix $A \in \mathbb{R}^{M \times N}$, $M \geq N$ has full column rank and let

$$A = U \begin{pmatrix} \Sigma & 0 \\ 0 & 0 \end{pmatrix} V^T = U_1 \Sigma V^T$$

be its singular value decomposition (SVD) [9, 32], where $U = (u_1, u_2, \ldots, u_M) = (U_1, U_2)$ and $V = (v_1, v_2, \ldots, v_N)$ are $M \times M$ and $N \times N$ orthogonal matrices, $U_1 = (u_1, u_2, \ldots, u_N)$ and $\Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_N)$ is diagonal. $\sigma_i, i = 1, 2, \ldots, N$, are called the singular values of $A$, $u_i$’s and $v_i$’s are the associated left and right singular vectors, respectively, and $(\sigma_i, u_i, v_i)$’s are called singular triplets. In this paper, slightly different from the convention, the singular values are labeled as $\sigma_1 \leq \sigma_2 \leq \cdots \leq \sigma_N$.

We are concerned with the following problem.

Problem 1. Compute numerically the $k$ smallest singular triplets $(\sigma_i, u_i, v_i)$ of $A$, $i = 1, 2, \ldots, k$, where $k \ll N$.

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There are many applications of Problem 1, including determination of numerical rank and of spectral condition number, least squares problems, total least squares problems, regression analysis, image and signal processing, pattern recognition and information retrieval, to name a few.

Consider the \((M+N)\times (M+N)\) augmented matrix
\[
\tilde{A} = \begin{pmatrix} 0 & A \\ A^T & 0 \end{pmatrix}.
\] (1.2)

Then, the eigenvalues of \(\tilde{A}\) are just \(\pm \sigma_1, \ldots, \pm \sigma_N\) and \(M-N\) zeros, the associated eigenvectors of \(\sigma_i\) and \(-\sigma_i\) are \(\frac{1}{\sqrt{2}} (u_i^T, v_i^T)^T\) and \(\frac{1}{\sqrt{2}} (u_i^T, -v_i^T)^T\), respectively, and the eigenvectors associated with zero eigenvalues have the form \((u_i^T, 0^T)^T\), where \(u_i\)'s are orthogonal to all \(u_1, \ldots, u_N\). Therefore, we obtain the following formulation of Problem 1.

**Problem 2.** Compute numerically the \(k\) smallest positive eigenvalues and the associated eigenvectors of \(\tilde{A}\). For the \(k\) smallest eigenpairs of \(\tilde{A}\), Problem 2 is a symmetric interior eigenvalue problem. Since \(M\) and \(N\) are assumed to be large, we can only resort to projection methods. A typical method is the symmetric Lanczos method [28]. It and other standard projection methods usually favor the extreme eigenvalues and the associated eigenvectors but are generally very inefficient for computing interior eigenpairs [28]. Another drawback is that in finite precision the computed eigenvalues do not come in plus-and-minus pairs and the computed eigenvectors do not respect the special structures that the true eigenvectors have.

Because of the mentioned drawbacks, we should not work on \(\tilde{A}\) explicitly for computing the smallest singular triplets of \(A\). Instead we attempt to solve Problem 1 directly by working on \(\tilde{A}\) implicitly. It appears that Lanczos bidiagonalization type methods [3, 11, 12, 20, 22, 24, 29] and Jacobi-Davidson SVD type methods [11, 12] can solve the mentioned problems elegantly. The Lanczos bidiagonalization type methods available have in common that they are all based on the Lanczos bidiagonalization process to build up orthonormal bases of certain Krylov subspaces. However, their mathematical backgrounds can be fundamentally different. Basically, there are three kinds of projection principles that extract different approximate singular triplets with respect to the subspaces. Some methods use the standard projection principle [2, 28, 32] to extract Ritz approximations [3, 4, 10, 11, 12, 20, 24, 29, 33], some methods use the harmonic projection principle [2, 32, 34] to extract harmonic Ritz approximations [3, 4, 11, 12, 22] and some methods use the refined projection principle [2, 13, 32, 34] to extract refined singular vector approximations [12, 20, 22]. Jacobi-Davidson type SVD methods for Problem 1 have several versions that are based on the three projection principles as well as their generalizations, respectively. As observed and claimed in [3, 12], the refined extraction version appears to give the best accuracy in general.

For Problem 1, due to the storage requirement and computational cost, all the Lanczos bidiagonalization type methods as well as Jacobi-Davidson type methods have to be restarted generally in order to make them converge. That is, for given projection subspaces, if the methods do not converge, then one repeatedly chooses new better starting vectors, constructs better subspaces and computes new approximate singular triplets until they converge. The implicit restarting technique due to Sorensen [30] is a powerful tool for restarting Krylov subspace algorithms in various contexts including large SVD problems [3, 4, 11, 12, 20, 22, 24, 29]. The success of an
implicitly restarted algorithm heavily depends on both the underlying method itself and a proper selection of the shifts involved; see, e.g., [15, 30]. Based on the Lanczos bidiagonalization method and one of its harmonic versions, Jia and Niu [20] and Larsen [24] have developed an implicitly restarted Lanczos bidiagonalization algorithm (IRLB), and Kokiopoulou et al. [22] have proposed an implicitly restarted harmonic Lanczos bidiagonalization algorithm (IRLANB) for computing the smallest singular triplets. IRLB uses the unwanted Ritz values and IRLANB uses the unwanted Ritz or harmonic Ritz values as shifts, respectively. These shifts are called exact shifts and harmonic shifts. Baglama and Reichel [3, 4] propose a thick restarting technique that explicitly augments small subspaces with certain Ritz or harmonic Ritz vectors, leading to augmented restarted Lanczos bidiagonalization algorithms (IRLBA). Hernández et al. [10] analyze a parallel implementation of this algorithm. Based on Stewart’s work for large eigenproblems [31], Stoll [33] presents a Krylov-Schur type algorithm that is restarted explicitly and is easily implemented.

It is shown in [20] that the Lanczos bidiagonalization method may fail to compute singular vectors though it converges for computing singular values for sufficiently good subspaces. To correct this deficiency, applying the refined projection principle proposed by the first author [13] (see also [2, 32, 34]), we have proposed a refined Lanczos bidiagonalization method, analyzed its convergence and developed an implicitly restarted refined Lanczos bidiagonalization algorithm (IRRLB) [20]. Based on the refined approximations to singular vectors, we have proposed refined shifts that are theoretically better than the exact shifts used within IRLB. Numerical experiments have demonstrated that IRRLB often outperforms IRLB [20, 24] considerably and is more efficient than several other available schemes: PROPACK [24], LANSO [23, 24], the MATLAB internal function svds and some others when computing the largest and smallest singular triplets.

Hochstenbach [11, 12] shows that for nested subspaces Ritz values approach the largest singular values monotonically but approach the smallest ones irregularly. So the Lanczos bidiagonalization method is more suitable for computing the largest singular triplets and may exhibit irregular convergence behavior when computing the smallest singular triplets. In contrast, the smallest harmonic Ritz values converge to the smallest singular values monotonically from above and may be better approximations. We continue to study how to compute the smallest singular triplets more efficiently in this paper. Based on the Lanczos bidiagonalization process, we propose a harmonic Lanczos bidiagonalization method by combining it with the harmonic projection principle. Our derivation is different from that in [3, 22]. The method is the same as that in [3] but different from the one in [22]. We prove that for good enough projection subspaces harmonic Ritz values converge if the columns of $A$ are strongly linearly independent. On the other hand, harmonic Ritz values may miss some desired singular values when the columns of $A$ are almost linearly dependent. So harmonic Ritz values may not be reliable. Furthermore, harmonic Ritz vectors may converge irregularly and even may fail to converge. These results imply that either implicitly or explicitly restarted algorithms may converge very slowly, converge irregularly or fail to converge. To circumvent these drawbacks, combining the harmonic projection principle with the harmonic projection principle, we propose a refined harmonic Lanczos bidiagonalization method that takes the Rayleigh quotients of harmonic Ritz vectors as more accurate and reliable approximate singular values and extracts the best approximations to the desired singular vectors from the given subspaces that minimize the residuals formed with the Rayleigh quotients. We prove
that refined harmonic Ritz approximations converge once the Krylov subspaces are good enough and the Rayleigh quotients converge. We then develop an implicitly restarted refined harmonic Lanczos bidiagonalization algorithm (IRRHLB). Based on the refined harmonic Ritz approximations to the desired singular vectors, in the spirit of Jia’s work [15, 17], we propose a new shifts scheme, called the refined harmonic shifts, that we show to be theoretically better than the harmonic shifts used within the implicitly restarted harmonic Lanczos bidiagonalization algorithm (IRHLB) and IRLANB. Motivated by [15, 17], we propose an efficient procedure to compute the refined harmonic shifts accurately.

It is worth noting that Kokiopoulou et al. [22] also use the refined projection principle to compute the refined harmonic Ritz approximations. They exploit the lower Lanczos bidiagonalization process, use the Ritz or harmonic Ritz values as shifts in the algorithm and compute the smallest singular triplets one by one by exploiting deflation. They only use the refined projection principle as refinement postprocessing at the end of each restart. The authors demonstrate that computing refined (harmonic) Ritz vectors and thus refined Ritz values benefits the overall convergence process. In particular, they show that while convergence is not apparent in terms of harmonic residual norms, monitoring refined residuals predicts convergence more accurately and safely. In contrast, based on the upper Lanczos bidiagonalization process and the refined projection principle, we propose a truly new method—the refined harmonic Lanczos bidiagonalization method that computes refined harmonic Ritz vectors as new approximations. We then develop IRRHLB with use of the new better shifts, called refined harmonic shifts, based on refined harmonic Ritz approximations. IRRHLB computes all the desired smallest singular triplets simultaneously.

The paper is organized as follows. In §2, based on the Lanczos bidiagonalization process, we derive the harmonic Lanczos bidiagonalization method and then present some basic and important properties of approximate singular vectors to be used later. Exploiting Jia’s results in [19], we then make a convergence analysis. In §3 we propose the refined harmonic Lanczos bidiagonalization method. We prove that the refined harmonic Ritz approximations converge for good enough subspaces once the Rayleigh quotients converge. In §4, we consider selection of the shifts involved. For IRHLB, similar to what is done in [3, 22], we use the harmonic Ritz values. For IRRHLB, by exploiting the available refined harmonic Ritz approximations, we propose the refined harmonic shifts that are proved to be theoretically better than the harmonic shifts. We then present an efficient procedure to compute them. We show that in finite precision the refined harmonic shifts can be computed accurately. Meanwhile, we extend the adaptive shifting strategy proposed by Larsen [24] and modified by Jia and Niu [20] to IRHLB and IRRHLB. In §5, we report numerical results and compare IRRHLB with the five other state of the art algorithms: IRHLB, IRLB, IRLANB and IRLBA, indicating that IRRHLB is at least competitive with the five other algorithms and can be considerably more efficient when computing the smallest singular triplets. Finally, we conclude the paper with some remarks in §6.

We introduce some notations to be used. Denote by \( \| \cdot \| \) the spectral norm of a matrix and the vector 2-norm, by \( \kappa(A) = \frac{\sigma_N}{\sigma_1} \), by \( K_m(C, v_1) = \text{span}\{v_1, Cv_1, \ldots, C^{m-1}v_1\} \) the \( m \)-dimensional Krylov subspace generated by the matrix \( C \) and the starting \( v_1 \), by the superscript ‘\( \text{T} \)’ the transpose of a matrix or vector, by \( I \) the identity matrix with the order clear from the context and by \( e_m \) the \( m \)-th coordinate vector of dimension \( m \).
2. The harmonic Lanczos bidiagonalization method and convergence.

Golub et al. [8] propose a Lanczos bidiagonalization method that can compute either the largest or the smallest singular triplets of $A$. The method is equivalent to the symmetric Lanczos method for the eigenproblem of $\tilde{A}$ starting with a special vector $[8, 28]$ and is based on the Lanczos bidiagonalization process [5, 9, 27], which satisfies the following relations if it does not break down before step $m$:

$$AQ_m = P_mB_m,$$
$$A^TP_m = Q_mB_m^T + \beta_m q_{m+1}e_m^T,$$  \hfill (2.1)  \hfill (2.2)

where the $m \times m$ matrix

$$B_m = \begin{pmatrix} \alpha_1 & \beta_1 \\ \alpha_2 & \ddots \\ \vdots & \beta_{m-1} \\ \alpha_m & \end{pmatrix},$$  \hfill (2.3)

and the columns of $Q_m = (q_1, q_2, \ldots, q_m)$ and $P_m = (p_1, p_2, \ldots, p_m)$ form orthonormal bases of the Krylov subspaces $K_m(A^TA, q_1)$ and $K_m(AA^T, p_1)$, respectively. So we have

$$P_m^TAQ_m = B_m.$$  \hfill (2.4)

The Lanczos bidiagonalization method computes the singular triplets $(\tilde{\sigma}_i, s_i, w_i)$, $i = 1, 2, \ldots, m$ of $B_m$ and then uses some of $(\tilde{\sigma}_i, P_m s_i, Q_m w_i)$, called the Ritz approximations, to approximate the largest and/or smallest singular triplets of $A$.

In finite precision, the columns of $P_m$ and of $Q_m$ may rapidly lose orthogonality. A partial reorthogonalization strategy [23, 24] is an effective technique for maintaining numerical orthogonality. However, Simon and Zha [29] show that it generally suffices to partially reorthogonalize only $P_m$ or $Q_m$ rather than reorthogonalizing them simultaneously. This may reduce the computational cost considerably when only reorthogonalizing the columns of $Q_m$ for $M \gg N$. In our codes, we adopt the strategy from [3] which is based on [29].

Given the subspace

$$E = \text{span} \left\{ \left( \begin{array}{cc} P_m & 0 \\ 0 & Q_m \end{array} \right) \right\},$$

the harmonic projection method of $\tilde{A}$ computes $(\tilde{\theta}_i, \tilde{\varphi}_i)$ satisfying the requirements

$$\tilde{\varphi}_i = \left( \begin{array}{c} P_m s_i \\ Q_m w_i \end{array} \right) \in E, \quad (\tilde{A} - \tilde{\theta}_i I)\tilde{\varphi}_i \perp AE$$  \hfill (2.5)

and uses them as approximations to some eigenpairs of $\tilde{A}$ [1, 32, 34].

Making use of (2.4), we see that (2.5) is equivalent to the generalized eigenproblem

$$\begin{pmatrix} 0 & B_m \\ B_m^T & 0 \end{pmatrix} \begin{pmatrix} s_i \\ w_i \end{pmatrix} = \frac{1}{\tilde{\theta}_i} \begin{pmatrix} B_m B_m^T + \beta_m e_m e_m^T & 0 \\ 0 & B_m^T B_m \end{pmatrix} \begin{pmatrix} s_i \\ w_i \end{pmatrix}.$$  \hfill (2.6)

$B_m$ is nonsingular as $A$ has full column rank and its singular values interlace those of $A$ [9, p. 449]. This is a symmetric generalized eigenvalue problem with one positive
definite matrix, so its eigenvalues are all real and nonzero [9, 32]. Furthermore, we present the following result.

**Theorem 2.1.** If \((\theta_i, s_i, w_i)\) satisfies (2.6), then \((-\theta_i, s_i, -w_i)\) or equivalently \((-\theta_i, -s_i, w_i)\) satisfies (2.6) too, that is, the eigenvalues of (2.6) come in plus-and-minus pairs and the eigenvectors have a special structure.

**Proof.** Equation (2.6) gives rise to

\[
B_m w_i = \frac{1}{\theta_i} \left( B_m B_m^T + \beta_m^2 e_m e_m^T \right) s_i,
\]
\[
B_m^T s_i = \frac{1}{\theta_i} B_m^T B_m w_i.
\]

So we can readily see that the assertion holds.

Assume that the nonnegative eigenvalues of (2.6) are ordered as

\[
0 \leq \theta_1 \leq \theta_2 \leq \cdots \leq \theta_{k+l},
\]

where \(k + l = m\). Then we use

\[
(\theta_i, \tilde{u}_i = P_m s_i / \|s_i\|, \tilde{v}_i = Q_m w_i / \|w_i\| = Q_m \tilde{w}_i), i = 1, 2, \ldots, k
\]

as approximations to the \(k\) smallest singular triplets \((\sigma_i, u_i, v_i)\). This method is called the harmonic Lanczos bidiagonalization method. \(\theta_i\)'s are called the harmonic Ritz values, \(\tilde{u}_i\)'s and \(\tilde{v}_i\)'s the (left and right) harmonic Ritz vectors, and \((\theta_i, \tilde{u}_i, \tilde{v}_i)\)'s the harmonic Ritz approximations. It is proved in [12] that

\[
\sigma_i \leq \theta_i, \ i = 1, 2, \ldots, m. \tag{2.8}
\]

We have the following basic and important properties, which will play a key role in §4.2.

**Theorem 2.2.** For \(i \neq j\) it holds that

\[
s_i^T B_m w_j = 0, \quad w_i^T B_m^T s_j = 0 \tag{2.9}
\]

and

\[
\tilde{u}_i^T A \tilde{v}_j = 0, \quad \tilde{v}_i^T A^T \tilde{u}_j = 0. \tag{2.10}
\]

**Proof.** Since (2.6) is a symmetric positive definite generalized eigenproblem, for \(i \neq j\) we have

\[
\begin{pmatrix}
  s_i^T \\
  w_i^T
\end{pmatrix}
\begin{pmatrix}
  0 & B_m \\
  B_m^T & 0
\end{pmatrix}
\begin{pmatrix}
  s_j \\
  w_j
\end{pmatrix} = 0,
\]

from which it follows that (2.9) holds.

(2.10) follows from \(\tilde{u}_i = P_m s_i / \|s_i\|, \quad \tilde{v}_i = Q_m w_i / \|w_i\|\) and (2.4). □

We now discuss efficient computation of harmonic Ritz approximations. It is disappointing that (2.6) is a \(2m \times 2m\) generalized eigenproblem. Fortunately, we can reduce (2.6) to a half sized SVD problem that can be solved more cheaply and accurately, as shown below.

We get from (2.6)

\[
(B_m B_m^T + \beta_m^2 e_m e_m^T) s_i = \theta_i B_m w_i, \tag{2.11}
\]

\[
B_m w_i = \theta_i s_i, \tag{2.12}
\]
from which it follows that

$$(B_mB_m^T + \beta^2_m e_m e_m^T)s_i = \theta_i^2 s_i.$$  \hfill (2.13)

So, the $(\theta_i, s_i)$'s are the singular values and right singular vectors of the $(m + 1) \times m$ matrix

$$\begin{pmatrix} B_m^T \\ \beta_m e_m^T \end{pmatrix}$$  \hfill (2.14)

and the left singular vectors

$$w_i = \theta_i B_m^{-1} s_i.$$  \hfill (2.15)

Therefore, we can get $(\theta_i, s_i)$ more accurately and efficiently by computing the SVD of the half sized (2.14) and obtain all the $w_i$'s by solving the bidiagonal linear systems $B_m w_i = \theta_i s_i$ at a total cost of $O(m^2)$ flops.

We comment that, based on the harmonic projection of $A^T A$ onto $K_m(A^T A, q_1)$, Baglama and Reichel \cite{3, 4} also derive (2.13)–(2.15). Our method is the same as that in \cite{3} but is different from the one in \cite{22}, which is based on the lower Lanczos bidiagonalization process.

From (2.1) and (2.2), we have

$$\|A\tilde{v}_i - \theta_i \tilde{u}_i\| = \|AQ_m \tilde{w}_i - \theta_i P_m \tilde{s}_i\| = \|P_m B_m \tilde{w}_i - \theta_i P_m \tilde{s}_i\| = \|B_m \tilde{w}_i - \theta_i \tilde{s}_i\|$$

and

$$\|A^T \tilde{u}_i - \theta_i \tilde{v}_i\| = \sqrt{\|B_m^T \tilde{s}_i - \theta_i \tilde{w}_i\|^2 + \beta_m^2 \|e_m^T \tilde{s}_i\|^2}.$$  \hfill (2.16)

Therefore, if

$$\sqrt{\|A\tilde{v}_i - \theta_i \tilde{u}_i\|^2 + \|A^T \tilde{u}_i - \theta_i \tilde{v}_i\|^2} = \sqrt{\|B_m \tilde{w}_i - \theta_i \tilde{s}_i\|^2 + \|B_m^T \tilde{s}_i - \theta_i \tilde{w}_i\|^2 + \beta_m^2 \|e_m^T \tilde{s}_i\|^2} < tol,$$

where $tol$ is a user prescribed accuracy, then the method is accepted as converged for $tol$.

We now analyze the convergence. Jia \cite{19} establishes a general convergence theory of harmonic projection methods for large eigenproblems. The theory can be adapted here.

From (2.6), set the matrices

$$\tilde{B} = \begin{pmatrix} 0 & B_m \\ B_m^T & 0 \end{pmatrix}$$

and

$$\tilde{C} = \begin{pmatrix} B_mB_m^T + \beta^2_m e_m e_m^T & 0 \\ 0 & B_m^T B_m \end{pmatrix}.$$  \hfill (2.17)

Recall from Theorem 2.1 that $\pm \theta_i$'s are the eigenvalues of $\tilde{B}^{-1} \tilde{C}$. The following result is direct from Theorem 2.1 and Corollary 2.2 of \cite{19}. 
There exists a perturbation matrix
\[ \sin \angle \left( \begin{pmatrix} u \\ v \end{pmatrix} , E \right) \]
value \( \sigma \) there always exists one harmonic Ritz value
it holds that
Then if
\[ \rho \]
quotient \( \rho \) small and the columns of \( \theta \) reliable, and
once the smallest singular value (Ritz value) of \( \tilde{A}^{-1} \tilde{C} \) may not be near zero, so that
So if \( \varepsilon \) is very small and the columns of \( A \) are strongly linearly independent.

To improve convergence and reliability of the method, we recommend the Rayleigh quotient \( \rho_i = \tilde{u}_i^T A \tilde{v}_i = \tilde{s}_i^T A \tilde{v}_i \), as a new approximation to \( \sigma_i \), as was also done in [12]. \( \rho_i \) is more accurate and reliable than \( \theta_i \). Correspondingly, \( \theta_i \) in (2.16) is replaced by \( \rho_i \). We refer to [19] for more theoretical results and arguments on such a replacement.

The following result is a direct application of Theorem 3.2 of [19].

**Theorem 2.4.** Let \( \theta, z = \begin{pmatrix} u \\ v \end{pmatrix} \) be an eigenpair of \( \tilde{A}^{-1} \tilde{C} \), and assume that \( Z \perp \) is such that the square matrix \( (z, Z \perp) \) is orthogonal and transforms \( \tilde{A}^{-1} \tilde{C} \) into
\[ \begin{pmatrix} z^T \\ Z_\perp^T \end{pmatrix} \tilde{A}^{-1} \tilde{C} (z, Z_\perp) = \begin{pmatrix} \theta & g^T \\ 0 & G \end{pmatrix} . \]

Then if
\[ \text{sep}(\sigma, G) > 0, \]
it holds that
\[ \sin \angle \left( \begin{pmatrix} u \\ v \end{pmatrix} , \begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix} \right) \leq \left( 1 + \frac{2\| \tilde{A}^{-1} \| \| A \|}{\sqrt{1 - \varepsilon^2 \text{sep}(\sigma, G)}} \right) \varepsilon \]
\[ \leq \left( 1 + \frac{2\| \tilde{A}^{-1} \| \| A \|}{\sqrt{1 - \varepsilon^2 (\text{sep}(\theta, G) - |\sigma - \theta|)}} \right) \varepsilon . \]
Theorem 2.4 states that if the separation sep(θ, G) of θ and the other harmonic Ritz values is uniformly bounded below by a positive constant then the harmonic Ritz approximations ˜u, ˜v converge. Unfortunately, however, for a general A, sep(θ, G) can be arbitrarily near zero, i.e., θ can be arbitrarily close to the other harmonic Ritz values. As a result, the upper bounds (2.21) and (2.22) can converge to zero very slowly and irregularly and even fail to do so as ε → 0. This means that the approximate singular vectors may converge very slowly and irregularly and even may fail to converge.

3. The refined harmonic Lanczos bidiagonalization method. The previous analysis shows that the harmonic Ritz approximations may converge slowly and irregularly and even may fail to converge. To overcome this intrinsic drawback, we now combine the harmonic Lanczos bidiagonalization method with the refined projection principle and derive a refined harmonic Lanczos bidiagonalization method. Recall that ρi = ˜sT Bm ˜wi. We use (ρi, ˜ψi) satisfying

\[
\begin{align*}
\tilde{\psi}_i &= \left( \begin{array}{c} p_m \\ q_m \\ x_i \\ y_i \\ e^T \\ \beta_m \\ \end{array} \right) \in E, \\
(\tilde{A} - \theta_i I)\tilde{\psi}_i &\perp \tilde{A}E, \\
\|\tilde{A}\tilde{\psi}_i - \rho_i \tilde{\psi}_i\| &= \min_{\psi \in E, \|\psi\| = 1} \|\tilde{A}\psi - \rho_i \psi\|
\end{align*}
\] (3.1)

to replace (θi, ˜ϕi) as a new approximation to an eigenpair of ˜A. The method first uses the harmonic Lanczos bidiagonalization method to compute (θi, ˜ϕi) and then forms the Rayleigh quotient ρi = ˜sT Bm ˜wi. With each ρi, i = 1, 2, . . . , k, it computes ψi by solving the minimization problem.

The following results adapted from [13, 17] can be used to compute ψi efficiently and accurately.

Theorem 3.1. Let z_i = (x_i^T, y_i^T)^T be the right singular vector of the matrix

\[
\begin{pmatrix}
0 & B_m \\
B_m^T & 0 \\
\beta_m e_m^T & 0
\end{pmatrix} - \rho_i \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}
\]

associated with its smallest singular value σ_min. Then

\[
\tilde{\psi}_i = \left( \begin{array}{c} p_m \\ 0 \\ q_m \\ 0 \end{array} \right) z_i,
\] (3.2)

\[
\|\tilde{A}\tilde{\psi}_i - \rho_i \tilde{\psi}_i\| = \sigma_{\text{min}}.
\] (3.3)

With ˜ψi at hand, we define the new left and right approximate singular vectors as

\[
\hat{u}_i = P_m x_i / \|x_i\| = P_m \hat{x}_i, \quad \hat{v}_i = Q_m y_i / \|y_i\| = Q_m \hat{y}_i
\] (3.4)

and use (ρi, ˜ui, ˜vi)’s to approximate the k smallest singular triplets of A. We call (ρi, ˜ui, ˜vi) a refined harmonic Ritz triplet and ˜ui, ˜vi a refined harmonic Ritz approximation.
Similar to (2.16), \((\rho_i, \hat{u}_i, \hat{v}_i)\) is accepted as converged if
\[
\sqrt{\|A\hat{v}_i - \rho_i\hat{u}_i\|^2 + \|A^T\hat{v}_i - \rho_i\hat{u}_i\|^2} = \sqrt{\|B_m\hat{y}_i - \rho_i\hat{x}_i\|^2 + \|B_m^T\hat{x}_i - \rho_i\hat{y}_i\|^2 + \beta_m^2|e_m\hat{x}_i|^2} \leq \text{tol.}
\]
(3.5)

The following result is taken directly from Theorem 4.1 of [21].

**Theorem 3.2.** Let \((\sigma, u, v)\) be a singular triplet of \(A\). Then there exist \(U_\perp\) and \(V_\perp\) such that \((u, U_\perp)\) and \((v, V_\perp)\) are orthogonal and
\[
\begin{pmatrix}
u^T \\ U_\perp^T
\end{pmatrix} A (v, V_\perp) = \begin{pmatrix}
\sigma & 0 \\
0 & L
\end{pmatrix},
\]
(3.6)
where \(L = U_\perp^T A V_\perp\). Set
\[
\tilde{L} = \begin{pmatrix}
0 & L \\ L^T & 0
\end{pmatrix}
\]
and assume that \((\rho, \hat{u}, \hat{v})\) is approximating \((\sigma, u, v)\). Then if
\[
\text{sep}(\rho, \tilde{L}) \geq \text{sep}(\sigma, \tilde{L}) - |\rho - \sigma| > 0,
\]
(3.7)
we have
\[
\sin \theta \left( \begin{pmatrix}
\hat{u} \\ \hat{v}
\end{pmatrix}, \begin{pmatrix}
u \\ v
\end{pmatrix} \right) \leq \frac{\|\tilde{A} - \rho L\| \varepsilon + |\rho - \sigma|}{\sqrt{1 - \varepsilon^2 \text{sep}(\sigma, L) - |\rho - \sigma|}}.
\]
(3.8)

Note that \text{sep}(\sigma, \tilde{L}) is the gap of \(\sigma\) and the other singular values of \(A\) and is a fixed constant. Theorems 3.2 shows that the refined harmonic Ritz approximations converge once \(\varepsilon \to 0\) and \(\rho \to \sigma\). Therefore, the refined harmonic Lanczos bidiagonalization method overcomes, to great extent, the possible non-convergence of the harmonic Ritz approximations.

4. The implicit restarting technique, shifts selection and an adaptive shifting strategy.

4.1. The implicit restarting technique. Due to the storage requirements and computational cost, in practice, the number of steps cannot be large and must be limited. For a relatively small \(m\), however, the \(m\)-dimensional subspaces \(K_m(A^T A, q_1)\) and \(K_m(A A^T, p_1)\), in general, do not contain enough information on the desired right and left singular vectors, so that both the harmonic and refined harmonic Lanczos bidiagonalization methods do not converge. Therefore, it is necessary to restart the methods. The idea is to repeatedly update new starting vectors based on the information available and construct increasingly better Krylov subspaces until the methods converge. Implicit restarting is usually preferable not only because of efficiency of the restart procedure, but also because the implicit procedure is more effective at locking in desired directions and purging unwanted ones.

We briefly review the implicit restarting technique for the Lanczos bidiagonalization process [6, 24]. Note that \(m = k + l\). After running \(l\) implicit QR iteration steps on \(B_m\) using the shifts \(\mu_j, j = 1, 2, \ldots, l\), we get
\[
\begin{align*}
\{ (B_m^T B_m - \mu_1^2 I) \cdots (B_m^T B_m - \mu_l^2 I) = \tilde{P} R, \\
\tilde{P}^T B_m Q \quad \text{upper bidiagonal},
\end{align*}
\]
(4.1)
where $\hat{P}$ and $\hat{Q}$ are the accumulations of Givens rotations applied to $B_m$ from the left and right, respectively. Define $Q_m^+ = Q_m \hat{Q}$, $P_m^+ = P_m \hat{P}$ and $B_m^+ = P_m^T B_m Q_m$. This process is achieved implicitly from $B_m^+ B_m$ to $(B_m^+)^T B_m^+$ by working on $B_m$ directly.

Performing the above $l$ implicit QR iteration steps gives the following relations [6]:

\[
A Q_k^+ = P_k^+ B_k^+, \quad (4.2)
\]

\[
A^T P_k^+ = Q_k^+ B_k^{+T} + (\beta_k \tilde{p}_{m,k} q_{m+1} + \beta_k q_{k+1}^+) v_k^+, \quad (4.3)
\]

where $\tilde{p}_{m,k}$ is the entry of $\hat{P}$ in position $(m,k)$ and the updated starting vector has the form

\[
\gamma q_1^+ = \prod_{j=1}^l (A^T A - \mu_j^2 I) q_1, \quad (4.4)
\]

with $\gamma$ a factor making $\|q_1^+\| = 1$. Since $\beta_k \tilde{p}_{m,k} q_{m+1} + \beta_k q_{k+1}^+$ is orthogonal to $Q_k^+$, we have obtained a $k$-step Lanczos bidiagonalization process starting with $q_1^+$. It is then extended to a $m$-step Lanczos bidiagonalization process in a standard way. So we avoid restarting the process from scratch and do it from step $k + 1$ upwards. This saves the computational cost of the first $k$ steps of the process. Applying the implicit restarting technique to the harmonic Lanczos bidiagonalization method and its refined version in such a way, we have formally sketched an implicitly restarted harmonic Lanczos bidiagonalization algorithm (IRHLB) and an implicitly restarted refined harmonic Lanczos bidiagonalization algorithm (IRRHLB).

4.2. Shifts selection. We can run IRHLB and IRRHLB once the shifts $\mu_1, \mu_2, \ldots, \mu_l$ are given. However, in order to make them work as efficiently as possible, we should select the best possible shifts in some sense for each algorithm. In the same spirit of [15, 17], it has been shown in [20] that if the shifts are more accurate approximations to some of the unwanted singular values of $A$ then the resulting subspaces contain more information on the desired singular vectors. The better the subspaces are, the faster IRHLB and IRRHLB may converge. For eigenproblems and SVD problems, Morgan [25, 26] and Kokiopoulou et al. [22] suggest using unwanted harmonic Ritz values as shifts, called the harmonic shifts here. These shifts are natural choices as they are the best approximations available to some of the unwanted eigenvalues and the unwanted singular values, respectively. So, for our IRHLB we also use the $l$ unwanted harmonic Ritz values $\theta_{k+1}, \theta_{k+2}, \ldots, \theta_m$ as shifts. Since the refined harmonic approximations $\tilde{u}_i, \tilde{v}_i$ are optimal in the sense of residual minimizations, they are generally more accurate than the harmonic Ritz approximations $\hat{u}_i, \hat{v}_i$. Therefore, based on $\hat{u}_i, \hat{v}_i$, $i = 1, 2, \ldots, k$, it should be possible to find better possible shifts than the harmonic shifts.

The following important result on the harmonic shifts is crucial for us to introduce and understand new better shifts for use within IRRHLB.

**Theorem 4.1.** Define

\[
\hat{U} = (\hat{u}_1, \ldots, \hat{u}_k), \quad \hat{V} = (\hat{v}_1, \ldots, \hat{v}_k),
\]

\[
\hat{U}_{\perp} = (\pm \hat{u}_{k+1}, \ldots, \pm \hat{u}_m), \quad \hat{V}_{\perp} = (\pm \hat{v}_{k+1}, \ldots, \pm \hat{v}_m).
\]

Then the harmonic shifts $\theta_{k+1}, \theta_{k+2}, \ldots, \theta_m$ are the absolute values of the $l$ harmonic Ritz values of $A$ with respect to the subspace span\{$(\hat{U}_{\perp}^T, \hat{V}_{\perp}^T)^T$\}. 


Proof. From definition (2.5) of the harmonic projection as well as the relationship between (2.5) and (2.6), it is easily verified that for \( i = k + 1, \ldots, m \), if the \( i \)-th column of \( \tilde{U}_\perp \) and that of \( \tilde{V}_\perp \) have the same or opposite \( \pm \) sign, then \( \tilde{A} \) has \( \theta_i \) or \(-\theta_i\) as one harmonic Ritz value with respect to the subspace \( \text{span}\{(\tilde{U}_\perp^T, \tilde{V}_\perp^T)^T\} \). 

We see from (2.10) that

\[
\tilde{U}^T A \tilde{V}_\perp = 0, \quad \tilde{V}^T A^T \tilde{U}_\perp = 0
\]

and

\[
\text{span}\{\tilde{V}\} \oplus \text{span}\{\tilde{V}_\perp\} = \text{span}\{Q_m\}, \quad \text{span}\{\tilde{U}\} \oplus \text{span}\{\tilde{U}_\perp\} = \text{span}\{P_m\}. \quad (4.5)
\]

Define \( \hat{U} = (\hat{u}_1, \ldots, \hat{u}_k) \) and \( \hat{V} = (\hat{v}_1, \ldots, \hat{v}_k) \), and let \( \hat{U}_\perp, \hat{V}_\perp \) be matrices with \( l = m - k \) columns satisfying

\[
\hat{U}^T A \hat{V}_\perp = 0, \quad \hat{V}^T A^T \hat{U}_\perp = 0 \quad (4.6)
\]

and

\[
\text{span}\{\hat{V}\} \oplus \text{span}\{\hat{V}_\perp\} = \text{span}\{Q_m\}, \quad \text{span}\{\hat{U}\} \oplus \text{span}\{\hat{U}_\perp\} = \text{span}\{P_m\}, \quad (4.7)
\]

where \( \oplus \) denotes the direct sum. Jia [18] derives a number of theoretical results that compare refined Ritz vectors and Ritz vectors. At this moment, we temporarily regard \( \tilde{A} \) as a general matrix, and \( \varphi_i, \hat{\varphi}_i \) are a Ritz and the corresponding refined Ritz vector of \( \tilde{A} \) with respect to a general subspace \( E \), respectively. One of Jia’s results says that we always have

\[
\|(\tilde{A} - \rho_i I) \hat{\varphi}_i\| < \|(\tilde{A} - \rho_i I) \varphi_i\|
\]

if the left-hand side is not zero and

\[
\|(\tilde{A} - \rho_i I) \hat{\varphi}_i\| \ll \|(\tilde{A} - \rho_i I) \varphi_i\|
\]

may occur if \( \rho_i \) is close to some \( \theta_j \) for \( j \neq i \). By standard perturbation theory in terms of residual norms, these two results demonstrate that \( \hat{\varphi}_i \) is generally more accurate and can be much more accurate than \( \varphi_i \). Here we should point out that these claims hold without requiring that \( E \) is sufficiently good. Jia [18] constructs a number of symmetric matrices having well separated simple eigenvalues and accurate subspaces to illustrate this. More precisely, assuming that \( \rho_i \) and \( \hat{\varphi}_i, \hat{\varphi}_i \) are used to approximate the eigenvalue \( \lambda_i \) and the eigenvector \( \varphi_i \) as one

\[
|\rho_i - \lambda_i| = O(\varepsilon), \quad \|(\tilde{A} - \rho_i I) \hat{\varphi}_i\| = O(\varepsilon), \quad \|(\tilde{A} - \rho_i I) \varphi_i\| = O(1).
\]

The above results are easily adapted to the harmonic and refined harmonic Ritz vectors. Some similar symmetric matrices are constructed by Jia in [19] for which the harmonic Ritz vectors have no accuracy at all but refined harmonic ones have accuracy \( O(\varepsilon) \). Coming back to our SVD context, the above results and analysis indicate that \( \tilde{u}_i \) and \( \tilde{v}_i \) are generally more accurate and can be much more accurate than \( \hat{u}_i \) and \( \hat{v}_i \) without the assumption that projection subspaces are sufficiently good.

Based on the above, it is evident that the subspaces \( \text{span}\{\hat{U}_\perp\} \) and \( \text{span}\{\hat{V}_\perp\} \) generally contain (possibly much) more accurate approximations to \( \pm u_i \) and \( \pm v_i \), \( i = k + 1, k + 2, \ldots, N \) than the subspaces \( \text{span}\{\tilde{U}_\perp\} \) and \( \text{span}\{\tilde{V}_\perp\} \) do. This, in turn,
means that the subspace \( \text{span}\{(\hat{U}_\perp, \hat{V}_\perp)^T\} \) contains (possibly much) more accurate approximations to the eigenvectors \( \frac{1}{\sqrt{2}}(a^T, \pm v)^T \) associated with the eigenvalues \( \pm \sigma_i, \ i = k + 1, k + 2, \ldots, N \), of \( \hat{A} \) than the subspace \( \text{span}\{(U_\perp, V_\perp)^T\} \) does. Recall from Theorem 2.3 that a better subspace should generally produce more accurate harmonic Ritz values. Hence, combining the above qualitative analysis with Theorem 4.1, we have come to the following key result.

**Proposition 4.2.** As approximations to some of \( \sigma_{k+1}, \ldots, \sigma_N \), the absolute values of the harmonic Ritz values \( \xi_i, i = 1, 2, \ldots, l \) of \( \hat{A} \) with respect to the subspace \( \text{span}\{(U_\perp, V_\perp)^T\} \) are generally more accurate and can be much more accurate than the harmonic shifts \( \theta_{k+1}, \theta_{k+2}, \ldots, \theta_m \).

This proposition holds without assuming that \( \text{span}\{Q_m\} \) and \( \text{span}\{P_m\} \) are sufficiently good. It suggests that we use better \( |\xi_i|, i = 1, 2, \ldots, l \) as shifts for use within \text{IRRHLB}. We call them the refined harmonic shifts.

Computationally, at first glance, it seems quite complicated and expensive to get the refined harmonic shifts as it involves constructing \( \hat{U}_\perp, \hat{V}_\perp \) that are related with the large \( A \). Inspired by the tricks in [15, 17], however, we can exploit (2.4) to propose an efficient procedure for computing them accurately, as shown below.

Recall (3.4) and define \( \hat{X} = (\hat{x}_1, \ldots, \hat{x}_k) \) and \( \hat{Y} = (\hat{y}_1, \ldots, \hat{y}_k) \). We use Householder transformations to compute the full QR decompositions

\[
B_m^T \hat{X} = Q_\perp \begin{pmatrix} R_X & 0 \\ 0 & 0 \end{pmatrix}, \quad B_m \hat{Y} = Q_\perp \begin{pmatrix} R_Y & 0 \\ 0 & 0 \end{pmatrix},
\]

which costs \( O(m^3) \) flops. Partition

\[
Q_X = (Q_X^1, Q_X^2), \quad Q_Y = (Q_Y^1, Q_Y^2),
\]

where \( Q_X^1 \) and \( Q_Y^1 \) are the first \( k \) columns of \( Q_X \) and \( Q_Y \), respectively, and let

\[
\hat{U}_\perp = P_m Q_Y^1, \quad \hat{V}_\perp = Q_m Q_X^2.
\]

Then it can be readily verified that

\[
\hat{U}_\perp^T A \hat{V}_\perp = \hat{X}^T P_m^T A Q_m Q_X^2 = \hat{X}^T B_m Q_X^2 = 0, \quad \hat{V}_\perp^T A^T \hat{U}_\perp = \hat{Y}^T Q_m^T A^T P_m Q_Y^2 = \hat{Y}^T B_m^T Q_Y^2 = 0.
\]

So \( \hat{U} \) and \( \hat{V} \) defined in this way meet conditions (4.6) and (4.7) and are just what we need. By (4.7), we have

\[
\text{span}\{\hat{U}\} = \text{span}\{P_m Q_Y^1\}, \quad \text{span}\{\hat{V}\} = \text{span}\{Q_m Q_X^1\}.
\]

The harmonic Ritz values \( \xi_i, i = 1, 2, \ldots, l \) of \( \hat{A} \) with respect to \( (\hat{U}_\perp, \hat{V}_\perp)^T \) satisfy

\[
(\hat{U}_\perp, \hat{V}_\perp)^T \hat{A} \begin{pmatrix} \hat{U}_\perp \\ \hat{V}_\perp \end{pmatrix} g_i = \frac{1}{\xi_i} (\hat{U}_\perp, \hat{V}_\perp)^T A \begin{pmatrix} \hat{U}_\perp \\ \hat{V}_\perp \end{pmatrix} g_i.
\]

Exploiting (2.4), we get a \( l \times l \) symmetric positive definite generalized eigenvalue problem

\[
\begin{pmatrix} Q_Y^1 & Q_X^2 \end{pmatrix} \begin{pmatrix} 0 & B_m^T \\ B_m & 0 \end{pmatrix} \begin{pmatrix} Q_Y^1 & Q_X^2 \end{pmatrix} g_i = \frac{1}{\xi_i} \begin{pmatrix} Q_Y^1 & Q_X^2 \end{pmatrix} \begin{pmatrix} B_m B_m^T + \beta_m^2 e_m e_m^T & 0 \\ 0 & B_m^T B_m \end{pmatrix} \begin{pmatrix} Q_Y^1 & Q_X^2 \end{pmatrix} g_i.
\]

\[\text{(4.12)}\]
The \( \xi \)'s are computed by the QZ algorithm \([9, 31]\) using \( O(l^3) \) flops. So the total cost of computing the refined harmonic shifts is \( O(m^3) \) flops, negligible compared with the harmonic Lanczos bidiagonalization method.

We give more details on computation of the refined harmonic shifts. Denote by \( F_m \) and \( G_m \) the matrices of the left and right-hand sides in (4.12), respectively, and observe that

\[
F_m = Q_{Y2}^T B_m Q_{X2} + Q_{X2}^T B_m^T Q_{Y2},
\]

\[
G_m = (B_m^T Q_{Y2})^T (B_m^T Q_{Y2}) + \beta_m^2 (e_m^T Q_{Y2}) (e_m^T Q_{Y2}) + (B_m Q_{X2})^T (B_m Q_{X2}).
\]  

(4.13)  

(4.14)

Noting that the two matrices in \( F_m \) are transposes each other, we only need to form \( Q_{Y2}^T B_m Q_{X2} \) by computing \( Q_{Y2}^T B_m \) or \( Q_{Y2}^T (B_m Q_{X2}) \), and \( Q_{Y2}^T B_m \) or \( B_m Q_{X2} \) is then used to form \( G_m \). Since \( G_m \) is symmetric, we only need to compute its upper triangular part. The total cost of forming \( F_m \) and \( G_m \) is \( O(m^3) \) flops. We then compute the eigenvalues \( 1/\hat{\xi} \)'s of the symmetric positive definite matrix pencil \( (F_m, G_m) \).

Now we show that in finite precision the above procedure is numerically stable and can compute the refined harmonic shifts accurately. There are three major steps in the procedure: the QR decompositions in (4.8), computation of \( F_m \) and \( G_m \) and the solution of the eigenvalue problem of \( (F_m, G_m) \) by the QZ algorithm. Note that the QR decompositions can be computed using Householder transformations in a numerically stable way (we use the Matlab built-in code qr in our implementation) and the QZ algorithm are numerically stable. Therefore, omitting details on roundoff errors, we finally compute the eigenvalues \( 1/\hat{\xi} \)'s of a perturbed matrix pencil \( (F_m + \delta F_m, G_m + \delta G_m) \), where \( \delta F_m \) and \( \delta G_m \) are the matrices of roundoff error accumulations and satisfy

\[
\frac{\|\delta F_m\|_F}{\|F_m\|_F}, \frac{\|\delta G_m\|_F}{\|G_m\|_F} = O(\epsilon_{\text{mach}})
\]  

(4.15)

with \( \epsilon_{\text{mach}} \) being the machine precision and \( \| \cdot \|_F \) the Frobenius norm.

For an eigenpair \( (\frac{1}{\xi}, g) \) of the pencil \((F_m, G_m)\) with \( \|g\| = 1 \), let \( \alpha = g^T F_m g \) and \( \beta = g^T G_m g \), so that \((\beta, \alpha)\) is a projective representation of the eigenvalue \( \frac{1}{\xi} \) \([32, \text{p. } 135]\). Then it is known \([32, \text{p. } 233]\) that there is an eigenvalue \( \frac{1}{\hat{\xi}} \) of the matrix pencil \((F_m + \delta F_m, G_m + \delta G_m)\) such that the chordal distance

\[
\chi(\frac{1}{\xi}, \frac{1}{\hat{\xi}}) \leq \sqrt{\frac{\|\delta F_m\|_F^2 + \|\delta G_m\|_F^2}{\alpha^2 + \beta^2}} + O(\epsilon_{\text{mach}}).
\]  

(4.16)

It is important to point out that for not too small \( \xi \) the chordal distance behaves like the ordinary distance \( |\xi - \hat{\xi}|\); see a remark in \([32, \text{p. } 140]\). So, how accurate \( \hat{\xi} \) is depends on the \( \frac{1}{\xi} \)'s condition number

\[
\nu = \frac{1}{\sqrt{\alpha^2 + \beta^2}}.
\]  

(4.17)

If one of \( \alpha \) and \( \beta \) is not small, \( \nu \) is not large and thus by (4.15) the relative error of \( \hat{\xi} \) is \( O(\epsilon_{\text{mach}}) \) if \( |\xi| \) is not very small.

We look at the smallest \( |\xi| \). By Proposition 4.2, it is known that the absolute values \( |\xi| \)'s better approximate some of \( \sigma_{k+1}, \ldots, \sigma_N \) than \( \theta_{k+1}, \ldots, \theta_m \). Furthermore,
recall from (2.8) that \( \theta_{k+1} \geq \sigma_{k+1} \). So if \( |\xi| \) and \( \theta_{k+1} \) both approximate \( \sigma_{k+1} \), then

\[
|\xi| - \sigma_{k+1} \lesssim (\theta_{k+1} - \sigma_{k+1}),
\]

so \( \sigma_{k+1} - (\theta_{k+1} - \sigma_{k+1}) \lesssim |\xi| \lesssim \sigma_{k+1} + (\theta_{k+1} - \sigma_{k+1}) \). Therefore, the smallest \( |\xi| \) is approximately bounded below by \( \sigma_{k+1} \).

In the following, we establish lower bounds for \( |\alpha| \) and \( |\beta| \) and an upper bound for \( \nu \) rigorously and prove when our proposed procedure can numerically compute the refined harmonic Ritz shifts accurately.

**Theorem 4.3.** For any refined harmonic Ritz shift \( \xi \), we have

\[
|\alpha| \geq 2\sigma_{k+1} \quad \text{and} \quad |\beta| \geq 2\sigma_{k+1}^2
\]  

(4.18)

and the \( \frac{1}{\xi} \)'s condition number is bounded from above:

\[
\nu \leq \frac{1}{2\sigma_{k+1} \sqrt{1 + \sigma_{k+1}^2}}.
\]  

(4.19)

If \( \sigma_{k+1} \) is not very small, then numerically the procedure described can compute the refined harmonic shifts \( |\xi| \)'s with relative accuracy \( O(\epsilon_{\text{mach}}) \).

**Proof.** From the definition of \( F_m \) and \( G_m \), we have

\[
|\alpha| = 2|y^T(Q_{Y2}^TB_mQ_{X2})g| \geq 2\sigma_{\min}(Q_{Y2}^TB_mQ_{X2}),
\]  

(4.20)

where \( \sigma_{\min}(C) \) denotes the smallest singular value of a matrix \( C \). Note that \( P_mQ_Y \) and \( Q_mQ_X \) form orthogonal bases of the left subspace \( \text{span}\{U\} \oplus \text{span}\{\hat{U}_\perp\} = \text{span}\{P_m\} \) and the right subspace \( \text{span}\{\hat{V}\} \oplus \text{span}\{\hat{V}_\perp\} = \text{span}\{Q_m\} \). Exploiting (2.4), (4.9), (4.10) and (4.11) and keeping in mind that \( \text{span}\{P_mQ_Y\} = \hat{U} \) and \( \text{span}\{Q_mQ_X\} = \text{span}\{\hat{V}\} \), we obtain from (4.6) that the projection matrix of \( A \) with respect to \( P_mQ_Y \) and \( Q_mQ_X \) is

\[
(P_mQ_Y)^T A(Q_mQ_X) = \begin{pmatrix}
Q_{Y1}^T P_{m}^T \\
Q_{Y2}^T P_{m}^T \\
\hat{U}_\perp^T
\end{pmatrix}
A(Q_mQ_X1, Q_mQ_X2)
= \begin{pmatrix}
Q_{Y1}^T P_{m}^T \\
\hat{U}_\perp^T
\end{pmatrix}
\begin{pmatrix}
0 \\
0 \\
0
\end{pmatrix}
= \begin{pmatrix}
Q_{Y1}^T B_mQ_{X1} \\
0 \\
0
\end{pmatrix}
= \begin{pmatrix}
Q_{Y1}^T B_mQ_{X1} \\
0 \\
0
\end{pmatrix}
\]

whose singular values \( \hat{\theta}_i \), \( i = 1, 2, \ldots, m \), labeled in increasing order, are the union of the singular values of \( Q_{Y1}^T B_mQ_{X1} \) and \( Q_{Y2}^T B_mQ_{X2} \) and are just the Ritz values of \( A \) with respect to the left and right subspaces \( \text{span}\{P_m\} \) and \( \text{span}\{Q_m\} \). By the singular value interlacing property, we have \( \sigma_i \leq \hat{\theta}_i \), \( i = 1, 2, \ldots, m \). Furthermore, note that \( Q_{Y1}^T B_mQ_{X1} \) and \( Q_{Y2}^T B_mQ_{X2} \) are the projection matrices of \( A \) with respect to the left subspaces \( \text{span}\{U\} \) and \( \text{span}\{\hat{U}_\perp\} \) and the right subspaces \( \text{span}\{\hat{V}\} \) and \( \text{span}\{\hat{V}_\perp\} \), respectively. Therefore, the singular values of \( Q_{Y1}^T B_mQ_{X1} \) are \( \hat{\theta}_i \), \( i = 1, 2, \ldots, k \) and approximate the \( k \) desired smallest singular values \( \sigma_i \)'s from above, while the singular values of \( Q_{Y2}^T B_mQ_{X2} = \hat{U}_\perp^T A\hat{V}_\perp \) are \( \hat{\theta}_i \), \( i = k+1, \ldots, m \) and approximate \( \sigma_{k+1}, \ldots, \sigma_m \) from above too. In particular, we have

\[
\hat{\theta}_{k+1} \geq \sigma_{k+1}.
\]
So it holds that
\[ |\alpha| \geq 2\sigma_{k+1}. \]

Next we estimate \( \beta \). We obtain from (4.14), (4.10) and (2.4)
\[
\beta = g^T(QY_2^TB_mB_m^TQY_2)g + \beta_m^2 g^T(QY_2^e_m e_m^TQY_2)g + g^T(QY_2^TB_mB_m^TQX_2)g \\
= g^T(\hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V)g + g^T(\hat{V}_V^T \hat{A}\hat{A}^T \hat{V}_V)g \\
\geq \sigma_{\min}(\hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V) + \sigma_{\min}(\hat{V}_V^T \hat{A}\hat{A}^T \hat{V}_V).
\]

Observe that \( \hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V \) and \( \hat{V}_V^T \hat{A}\hat{A}^T \hat{V}_V \) are the projection matrices of \( \hat{A}\hat{A}^T \) and \( \hat{A}^T \hat{A} \) with respect to \( \text{span}\{\hat{U}_V\} \) and \( \text{span}\{\hat{V}_V\} \), respectively. So their eigenvalues approximate some of the eigenvalues \( \sigma_{k+1}^2, \ldots, \sigma_N^2 \) of \( \hat{A}\hat{A}^T \) and \( \hat{A}^T \hat{A} \). Furthermore, since
\[
\hat{V}_V^T \hat{A}\hat{A}^T \hat{V}_V - (\hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V)^T(\hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V) = \hat{V}_V^T \hat{A}(I - \hat{U}_V^T \hat{U}_V)\hat{A}^T \hat{V}_V,
\]
is symmetric nonnegative definite, the smallest eigenvalue of \( \hat{V}_V^T \hat{A}\hat{A}^T \hat{V}_V \) is no less than the smallest eigenvalue \( \hat{q}_{k+1}^2 \) of \( (\hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V)^T(\hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V) \). As a consequence, it follows from \( \hat{q}_{k+1} \geq \sigma_{k+1} \) that the smallest eigenvalue of \( \hat{V}_V^T \hat{A}\hat{A}^T \hat{V}_V \) is bounded below by \( \sigma_{k+1}^2 \).

Similarly, we have
\[
\hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V - (\hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V)^T(\hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V) = \hat{U}_V^T \hat{A}(I - \hat{V}_V^T \hat{V}_V)\hat{A}^T \hat{U}_V,
\]
which is symmetric nonnegative definite. As a result, the smallest eigenvalue of \( \hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V \) is no less than the smallest eigenvalue \( \hat{q}_{k+1}^2 \) of \( (\hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V)^T(\hat{U}_V^T \hat{A}\hat{A}^T \hat{U}_V) \) and is bounded below by \( \sigma_{k+1}^2 \). Therefore, we get
\[ \beta \geq 2\sigma_{k+1}^2. \]

So it follows from (4.18) that the \( \frac{1}{\xi} \)'s condition number \( \nu \) in (4.17) satisfies
\[ \nu \leq \frac{1}{2\sigma_{k+1} \sqrt{1 + \sigma_{k+1}^2}}, \]
which is (4.19).

If \( \sigma_{k+1} \) is not very small, then \( \nu \) is not large and all \( \xi \)'s are not too small. Keep in mind the comments on (4.15) and (4.16). It is then clear that numerically the proposed procedure can compute the refined harmonic shifts \( [\xi_i] \)'s with relative accuracy \( O(\epsilon_{\text{mach}}) \).

We should point out that Theorem 4.3 holds without any assumption on \( \text{span}\{Q_m\} \) and \( \text{span}\{P_m\} \), as is clearly seen from the proof.

### 4.3. Adaptive shifting strategy

It has been observed [24] that if the \( k \)-th desired \( \sigma_k \) is very near a shift then IRLB with the exact shifts (the unwanted Ritz values) converges very slowly and even stagnates. This is also the case for IRRHLB with the refined harmonic shifts and IRRHLB with the harmonic shifts. The reason is that if some shift \( \mu_i \) is very near \( \sigma_k \) then the new starting vector \( q_k^+ \) will nearly annihilate the component of the desired \( v_k \), so that the new subspace \( \mathcal{K}_m(A^T A, q_k^+) \) contains very little information on \( v_k \) and \( \rho_k \) converges to \( \sigma_k \) very slowly or not at all.

In order to overcome this problem, for IRLB with the exact shifts, Larsen [24] proposes an adaptive shifting strategy for computing the largest singular triplets. He
simply replaces a bad shift to be defined below by a zero shift. Jia and Niu [20] adapt it to IRRLB for computing the largest singular triplets but modify it for computing the smallest singular triplets. Their strategy works for IRHLB and IRRHLB: Define the relative gaps of \( \rho_k \) and all the shifts \( \mu_i \), \( i = 1, 2, \ldots, l \) by

\[
\text{relgap}_{ki} = \left| \frac{(\rho_k - \varepsilon_k) - \mu_i}{\rho_k} \right|, \tag{4.21}
\]

where \( \varepsilon_k \) is the residual norm (2.16) or (3.5). We should note that \( \rho_k - \varepsilon_k \) is an approximation to \( \sigma_k \). If \( \text{relgap}_{ki} \leq 10^{-3} \), \( \mu_i \) is a bad shift and should be replaced by a suitable quantity.

Expand \( q_1 \) as a linear combination of the right singular vectors \( \{v_j\}_{j=1}^N \):

\[
q_1 = \sum_{j=1}^N \alpha_j v_j.
\]

Then for the harmonic shifts \( \mu_i = \theta_{k+1} + i, i = 1, 2, \ldots, l \) we have from (4.4)

\[
\gamma q_1^+ = \prod_{i=k+1}^m (A^T A - \theta_i^2 I) q_1
\]

\[
= \sum_{j=1}^k \alpha_j \prod_{i=k+1}^m (\sigma_j^2 - \theta_i^2) v_j + \sum_{j=k+1}^N \alpha_j \prod_{i=k+1}^m (\sigma_j^2 - \theta_i^2) v_j,
\]

So if \( \theta_{k+1} \) is very near \( \sigma_k \), which is the case that \( \sigma_{k+1} \) is very near \( \sigma_k \), then \( q_1^+ \) has a very small component in the direction of \( v_k \). A good strategy is to replace \( \theta_{k+1} \) by the largest one among all the shifts, as this strategy amplifies the components of \( q_1^+ \) in \( v_i, i = 1, 2, \ldots, k \) and meanwhile dampens those in \( v_i, i = k + 1, \ldots, N \).

The above strategy applies to the refined harmonic shifts as well.

We now present IRHLB with the harmonic shifts and IRRHLB with the refined harmonic shifts, respectively.

**Algorithm 1. IRHLB with the harmonic shifts**

1. Given a unit length starting vector \( q_1 \) of dimension \( N \), the steps \( m \), the number \( k \) of the desired singular triplets and the convergence tolerance \( \text{tol} \).
2. Run the \( m \)-step Lanczos bidiagonalization process and construct \( B_m, P_m \) and \( Q_m \).
3. Calculate the triplets \( (\theta_i, \tilde{s}_i, \tilde{w}_i), i = 1, 2, \ldots, m \), by computing the singular values and right singular vectors of (2.14) and by solving (2.15) and normalizing the solutions, and use the Rayleigh quotients \( \rho_i = \tilde{u}_i^T A \tilde{v}_i = \tilde{s}_i^T B_m \tilde{w}_i \) as approximations to \( \sigma_i, i = 1, 2, \ldots, k \).
4. Replace \( \theta_i \) by \( \rho_i \) in (2.16). For \( i = 1, 2, \ldots, k \), test if (2.16) is satisfied. If yes, compute \( \tilde{u}_i \) and \( \tilde{v}_i \) explicitly and stop.
5. Implicitly restart the Lanczos bidiagonalization process using the harmonic shifts and the adaptive shifting strategy.

**Algorithm 2. IRRHLB with the refined harmonic shifts**

1. Given a unit length starting vector \( q_1 \) of dimension \( N \), the steps \( m \), the number \( k \) of the desired singular triplets and the convergence tolerance \( \text{tol} \).
2. Run the \( m \)-step Lanczos bidiagonalization process and construct \( B_m, P_m \) and \( Q_m \).
3. Calculate the triplets \((\theta_i, \tilde{s}_i, \tilde{w}_i), i = 1, 2, \ldots, m\) by computing the singular values and right singular vectors of (2.14) and by solving (2.15) and normalizing the solutions, and use the Rayleigh quotients \(\rho_i = \tilde{u}_i^T A \tilde{v}_i = \tilde{s}_i^T B_m \tilde{w}_i\) as approximations to \(\sigma_{1,1}, \sigma_{2,1}, \ldots, \sigma_{k,1}\).

4. For each \(\rho_i, i = 1, 2, \ldots, k\), compute \(\hat{x}_i\) and \(\hat{y}_i\) in Theorem 3.1.

5. For \(i = 1, 2, \ldots, k\), test if (3.5) is satisfied. If yes, compute \(\hat{u}_i\) and \(\hat{v}_i\) by (3.4) explicitly and stop.

6. Implicitly restart the Lanczos bidiagonalization process using the refined harmonic shifts and the adaptive shifting strategy.

5. **Numerical experiments.** We have developed the experimental Matlab codes of IRRHLB, IRHLB, IRRLB and IRLB. The latter two were named IRRBL and IRBL in [20] and were originally developed based on the lower Lanczos bidiagonalization process. Here we have developed their upper Lanczos bidiagonalization versions. These four codes call the upper Lanczos bidiagonalization process in Baglama and Reichel’s code IRLBA, and some parameters and defaults are the same as those used in IRLBA. We compare IRRHLB with IRRHLB, IRHLB, IRLB, IRLBA and IRLANB in this section and report numerical results. Numerical experiments were run on an Intel Core 2 E6320 with CPU 1.86GHz and RAM 2GB under the Window XP operating system using Matlab 7.1 with \(\epsilon_{\text{mach}} = 2.22 \times 10^{-16}\). The stopping criteria are

\[
\text{stopcrit} = \max_{1 \leq i \leq k} \sqrt{\| A \tilde{u}_i - \rho_i \hat{u}_i \|^2 + \| A^T \tilde{v}_i - \rho_i \hat{v}_i \|^2} \quad \text{IRRHLB}
\]

and

\[
\text{stopcrit} = \max_{1 \leq i \leq k} \sqrt{\| A \tilde{u}_i - \rho_i \hat{u}_i \|^2 + \| A^T \tilde{v}_i - \rho_i \hat{v}_i \|^2} \quad \text{IRRHLB}
\]

If

\[
\text{stopcrit} = \frac{\text{stopcrit}}{\| A \|} < \text{tol},
\]

then stop. Similar criteria apply to IRLB and IRRLB as well. In (5.1), \(\| A \|\) is replaced by the maximum of the current largest (harmonic) Ritz value and the old one obtained at last restart. Some parameters in IRRHLB, IRHLB, IRRLB and IRLB are described in Table 5.1.

For large matrix eigenproblems, in order to speed up convergence, ARPACK (eigs) and Implicitly Restarted Refined Arnoldi Method (IRRA) [15] compute \(k+3\) approximate eigenpairs, so the number of shifts is \(m - (k + 3)\) when \(k\) eigenpairs are desired. This strategy adapts to Krylov type subspace algorithms for SVD problems, for instance, the default parameter \(\text{adjust} = 3\) in IRLBA, which means that the updating subspaces are augmented with \(k+3\) Ritz or harmonic Ritz vectors. With \(m - (k + 3)\) exact shifts and harmonic shifts used, IRLB, IRHLB and IRLANB retain \(k+3\) Ritz vectors and harmonic Ritz vectors in the updating subspaces, respectively.

We mention that our codes IRRHLB, IRHLB, IRRLB and IRLB as well as IRLBA and IRLANB (we used the newest available code \textit{irlanb\_review}) do not involve any shift-and-invert matrix when computing the smallest singular triplets, while the Matlab internal function \texttt{svds} needs to factorize \(\tilde{A}\) of (1.2). In this context, we assume that \(A\) is too large to allow any factorization of \(\tilde{A}\) due to excess memory and/or computational cost, so we do not compare the above six algorithms with \texttt{svds}.\]
Table 5.1
Parameters in IRRHLB, IRRLB, IRHLB and IRLB

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k )</td>
<td>Number of the desired singular triplets. Default value: ( k = 6 ).</td>
</tr>
<tr>
<td>( \text{adjust} )</td>
<td>Number added to ( k ) to speed up convergence. Default value: ( \text{adjust} = 3 ).</td>
</tr>
<tr>
<td>( \text{disps} )</td>
<td>When ( \text{disps} &gt; 0 ), the ( k ) desired approximate singular values and norms of associated absolute residual error are displayed each iteration. ( \text{disps} = 0 ) inhibits display of these quantities. Default value: ( \text{disps} = 1 ).</td>
</tr>
<tr>
<td>( M_B )</td>
<td>Maximum of Lanczos bidiagonalization steps. Default value: ( M_B = 20 ).</td>
</tr>
<tr>
<td>( \text{maxit} )</td>
<td>Maximum number of restarts. Default value: ( \text{maxit} = 300 ).</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>A 2-letter string which specifies which extreme singular triplets are to be computed, ‘SS’ for the smallest and ‘LS’ for the largest. Default value: ( \sigma = \text{‘SS’} ).</td>
</tr>
<tr>
<td>( \text{tol} )</td>
<td>User defined relative tolerance to check convergence. Default value: ( \text{tol} = 10^{-6} ).</td>
</tr>
<tr>
<td>( v_0 )</td>
<td>( \min(M, N) )-dimensional initial vector of Lanczos bidiagonalization. Default value: ( v_0 = \text{randn}(\min(M, N), 1) ).</td>
</tr>
</tbody>
</table>

Our experiments consist of three subsections. In the first two subsections, we test IRRHLB on a set of matrices having clustered smallest singular values and on a set of ill-conditioned matrices, respectively. We show that IRRHLB works well on them and confirm some theory. In the third subsection, we compare IRRHLB with the five other algorithms on seven practical problems that include very difficult, difficult and general ones, illustrating that IRRHLB is at least competitive with and can be much more efficient than the five other algorithms.

5.1. IRRHLB for the clustered smallest singular values. This set of experiments is designed to see how IRRHLB behaves for the clustered smallest singular values. Similar to those matrices in [22], we constructed a sequence of diagonal matrices \( A_s \in \mathbb{R}^{n \times n} \), \( n = 1000 \), \( s = 1, \ldots, 4 \) whose nine smallest singular values become increasingly more clustered as \( s \) increases. In the Matlab language:

\[
A_s = spdiags([1 : 10^{-8} : 1 + 9 \times 10^{-4}, 2 : 1 : 1000]', [0, 1000, 1000], s = 1, \ldots, 4, \quad (5.2)
\]

whose smallest singular value \( \sigma_1 = 1 \) and \( \kappa(A_s) = 991 \) for all \( s \). Since \( \kappa(A_s) \) is moderate, it is expected that IRRHLB computes \( \sigma_1 \) accurately if it works. We computed \( \sigma_1 \) by taking the parameters

\[
\text{opts.m} = 50, \text{opts.maxit} = 2000, \text{opts.adjust} = 9, \text{opts.tol} = 1e-8
\]

and using the same starting vector generated randomly in a normal distribution for all \( s \). Figure 5.1 plots absolute residual norms of the computed singular triplets and relative errors \( |\rho - 1| \), respectively. We see that IRRHLB succeeded for all \( s \) and computed the smallest singular value accurately. In the worst case \( s = 4 \), IRRHLB gave the relative error \( |\rho - 1| = 3.7 \times 10^{-8} \), the same order as the backward error that
Fig. 5.1. Experiments with the matrices (5.2), with the clustering smallest singular value. Solid lines correspond to residual norms. Dotted lines to relative errors of the smallest singular value computed by IRRHLB.

equals the relative residual norm $10^{-8}$. For $s = 3$, the relative error $|\rho - 1| = 3.5 \times 10^{-9}$. Both are in agreement with the standard perturbation theory [9, 31]. For $s = 1, 2$, the relative errors $|\rho - 1|$ are $1.3 \times 10^{-12}$ and $8.1 \times 10^{-14}$, respectively, a few order smaller than the predicted relative error $O(10^{-8})$. Also, IRRHLB used considerably fewer restarts for $s = 1$ than for the other bigger $s$ but had comparable restarts for $s = 2, 3, 4$. It was expected that IRRHLB converged faster for $s = 1$ than for $s = 2, 3, 4$ since the gap of $\sigma_1$ and $\sigma_2$ is considerably bigger for $s = 1$ than those for $s = 2, 3, 4$.

5.2. IRRHLB for ill-conditioned matrices. We investigate the behavior of IRRHLB for a set of ill-conditioned matrices. Similar to those matrices in [22], we constructed a sequence of bidiagonal matrices $A_s \in \mathbb{R}^{n \times n}$, $n = 1000$, $s = 4, \ldots, 7$ and $9, \ldots, 12$ with increasing condition numbers:

$$A_s = \text{spdiags}([\text{linspace}(1, 10^s, 1000)' \cdot 0, 1000, 1000]),$$

(5.3)

whose smallest singular value $\sigma_1 = 1$ and condition numbers $\kappa(A_s) = 10^s$. We computed $\sigma_1$ by taking the parameters

$$\text{opts.m} = 50, \text{opts.maxit} = 2000, \text{opts.adjust} = 3, \text{opts.tol} = 1e - 14$$

using the same starting vector generated randomly in a normal distribution for all $s$. Figure 5.2 plots relative errors $|\rho - 1|$. It was seen from the figure that IRRHLB
computed the smallest singular value with relative error smaller than $10^{-8}$ for $s = 4, 5, 6, 7$. This confirms the perturbation theory: the smaller $s$ is, the smaller the relative error is. For more ill-conditioned cases $s = 9, 10, 11, 12$, the accuracy of the computed smallest singular values deteriorated significantly. For $s = 9, 10$, the relative errors are $9.0 \times 10^{-5}$ and $4.0 \times 10^{-5}$, and the computed singular values have four and five correct decimal digits, respectively. In the worst-conditioned case that $s = 12$, the relative error is 0.3848; for $s = 11$, the relative error is 0.1678, and the computed smallest singular value was a little bit more accurate than that for $s = 12$.

We also tested $\texttt{opts.tol} = 1e - 12$ and compared the results with those for $\texttt{opts.tol} = 1e - 14$. We found that although residual norms continued decreasing until $10^{-14}$, the accuracy of the computed singular values was not improved further as residual norms decreased from $\texttt{opts.tol} = 1e - 12$ to $\texttt{opts.tol} = 1e - 14$. This was reflected by the figures, where we saw that relative errors did not decrease further and stabilized, starting from some restart for each $s$ except $s = 9$. The curves for $s = 9$ jumped up and down when the algorithm approached convergence, but kept below $10^{-4}$. All these are in accordance with the predicted relative errors, which should not be bigger than a very modest multiple of $\kappa(A_s) \times \texttt{opts.tol}$. Another important observation is that IRRHLB used more restarts as $s$ increases. Since the ratio $\frac{\sigma_2 - \sigma_1}{\sigma_2 - \sigma_1}$, the spread over the gap of $\sigma_1$ and $\sigma_2$, increases as $s$ does, it is more difficult for IRRHLB to solve the SVD problem as $s$ increases. We also saw that the curves of relative errors oscillated quite often in the middle of convergence processes. A careful observation revealed that IRRHLB started to be on its way to compute the desired singular value at some stage but lost it soon. Then it adaptively adjusted convergence repeatedly and eventually was on the correct way to converge. These phenomena may be explained by Theorem 2.3 and the comments that follow it.

![Fig. 5.2. Experiments with the increasingly ill-conditioned diagonal matrices (5.3), with $\kappa(A_s) = 10^s$, $s = 4, 5, 6, 7, 9, 10, 11, 12$.](image)

### 5.3. Experiments of the six algorithms on practical problems

We now do numerical experiments on several selected problems that include very difficult, difficult and general ones. We compare IRRHLB with the five other algorithms: IRRLB, IRHLB, IRLB, IRLBA and IRLANB.

Table 5.2 lists seven test matrices from [1, 7] and some of their basic properties. Except well1852, all other matrices are square matrices. Note that the ratio $\frac{\text{spread}(A)}{\text{gap}(A)}$ indicates whether or not the six algorithms have difficulty converging. The bigger
is, the more slowly the algorithms converge generally. From the table, we see that the \( k (= 1, 3, 5, 10) \) desired smallest singular values of all the matrices are quite clustered; among them the matrices fidap4, jagmesh8 and lshp3025 are the most difficult, the matrix plat1919 is relatively difficult, and the matrices well1850 and dw2048 are general. We see that all \( \kappa(A) \)'s are not very large, so the columns of \( A \) are strongly linearly independent. It is expected that if the algorithms converge then they can compute the smallest singular values with relative errors no more than a very modest multiple of \( \kappa(A) \times \text{opts.tol} \).

### Table 5.2

<table>
<thead>
<tr>
<th>Matrix</th>
<th>fidap4</th>
<th>jagmesh8</th>
<th>lshp3025</th>
<th>well1850</th>
<th>dw2048</th>
<th>pde2961</th>
<th>plat1919</th>
</tr>
</thead>
<tbody>
<tr>
<td>nnz((A))</td>
<td>31837</td>
<td>7465</td>
<td>20833</td>
<td>8755</td>
<td>10114</td>
<td>14580</td>
<td>32399</td>
</tr>
<tr>
<td>(\kappa(A))</td>
<td>2.4e + 3</td>
<td>2.2e + 4</td>
<td>6.8e + 4</td>
<td>1.1e + 2</td>
<td>2.1e + 3</td>
<td>6.4e + 2</td>
<td>3.7e + 2</td>
</tr>
<tr>
<td>spread((A))</td>
<td>1.6e + 0</td>
<td>6.8e + 0</td>
<td>7.0e + 0</td>
<td>1.8e + 0</td>
<td>9.8e - 1</td>
<td>1.0e + 1</td>
<td>2.3e + 0</td>
</tr>
<tr>
<td>gap(1)</td>
<td>1.5e - 3</td>
<td>1.7e - 3</td>
<td>1.8e - 3</td>
<td>3.0e - 3</td>
<td>2.6e - 3</td>
<td>8.2e - 3</td>
<td>2.6e - 3</td>
</tr>
<tr>
<td>gap(3)</td>
<td>2.5e - 4</td>
<td>1.6e - 3</td>
<td>9.1e - 4</td>
<td>3.0e - 3</td>
<td>2.9e - 4</td>
<td>2.4e - 3</td>
<td>1.8e - 3</td>
</tr>
<tr>
<td>gap(5)</td>
<td>2.5e - 4</td>
<td>4.8e - 5</td>
<td>1.8e - 4</td>
<td>3.0e - 3</td>
<td>2.9e - 4</td>
<td>2.4e - 3</td>
<td>2.7e - 4</td>
</tr>
<tr>
<td>gap(10)</td>
<td>2.5e - 4</td>
<td>4.8e - 5</td>
<td>2.2e - 5</td>
<td>2.6e - 3</td>
<td>1.6e - 4</td>
<td>5.2e - 4</td>
<td>2.0e - 4</td>
</tr>
</tbody>
</table>

We computed the \( k \) smallest singular triplets for different \( k \). To make a reasonable comparison, for each matrix except well1850 we used the same starting vector generated randomly in a normal distribution for the six algorithms. For well1850, we took the same starting vector \( v_0 = \text{randn}(1850,1) \) in IRLANB and the same starting vector \( v_0 = \text{ran}\text{d}(712,1) \) in the five other algorithms. In all tables, denote by \( \text{iter} \) the number of restarts, by \( \text{time} \) CPU time in second, by \( \text{n.c} \) non-convergence after 2000 restarts are used, and by \( \text{mv} \) the number of matrix-vector products. Since matrix-vector products involving \( A \) are equal to those involving \( A^T \), we only count the number of matrix-vector products involving \( A \). We compare restarts and matrix-vector products as well as CPU time needed by all the codes for the same \( k \) and \( m \). The former two quantities reflect the overall efficiency of the codes more fairly and reasonably.

By the above description, in IRHLB, IRRLB, IRHLB, IRLB and IRLBA we took the input parameters

\[
\text{opts.k} = k, \text{opts.M.B} = m, \text{opts.tol} = \text{tol}, \text{opts.maxit} = 2000, \text{opts.v0} = v_0
\]

and the others as defaults. In IRLANB we took

\[
\text{eignum} = k, \text{options.k} = m - 1, \text{options.l} = m - 1 - (k + 3), \\
\text{options.u0} = v_0, \text{options.maxit} = 2000, \text{options.version} = '\text{harmonic}'
\]

and the others as defaults. This parameters make all the codes compute the approximate singular triplets with respect to certain subspaces of the same dimension \( m \) and use the same number of shifts at each restart.

We found that fidap4, jagmesh8 and lshp3025 challenged most of the six algorithms. Tables 5.3–5.5 report the results obtained by IRRHLB and IRRLB for \( \text{opts.tol} = 1e - 6 \).
A REFINED HARMONIC LANCZOS BIDIAgonALIZATION METHOD

Table 5.3

<table>
<thead>
<tr>
<th>$k = 1$</th>
<th>$m = 15$</th>
<th>$m = 20$</th>
<th>$m = 25$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method</td>
<td>iter</td>
<td>time</td>
<td>mv</td>
</tr>
<tr>
<td>IRRHLB</td>
<td>807</td>
<td>46.5</td>
<td>8881</td>
</tr>
<tr>
<td>IRRLB</td>
<td>n.c</td>
<td>-</td>
<td>-</td>
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<table>
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<th>$m = 25$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method</td>
<td>iter</td>
<td>time</td>
<td>mv</td>
</tr>
<tr>
<td>IRRHLB</td>
<td>1083</td>
<td>55.4</td>
<td>9753</td>
</tr>
<tr>
<td>IRRLB</td>
<td>n.c</td>
<td>-</td>
<td>-</td>
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</tbody>
</table>

Table 5.4

<table>
<thead>
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<th>$m = 20$</th>
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<th>$m = 30$</th>
</tr>
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<tbody>
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<td>Method</td>
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<td>time</td>
<td>mv</td>
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<td>-</td>
<td>-</td>
</tr>
<tr>
<td>IRLB</td>
<td>n.c</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>IRLBA</td>
<td>n.c</td>
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Clearly, for fidap4 and lshp3205, IRRHLB worked well and solved the problem successfully while IRRLB only performed well in some cases and was less efficient than IRRHLB. In contrast, IRRHLB, IRLB, IRLBA and IRLANB performed more poorly and they all failed to converge for fidap4 and lshp3205. For jagmesh8, IRRHLB still worked robustly and efficiently, but IRRLB succeeded only in a few cases and IRRHLB, IRLB, IRLBA and IRLANB behaved more badly. They all were considerably less efficient than IRRHLB if they worked. We found that, generally, the bigger $k$ was, the more restarts IRRHLB and IRRLB used for the same $m$. This should not be surprising as the problem for a bigger $k$ is generally more difficult to solve than that for a smaller $k$. We also observed that all the smallest singular values were computed with relative errors no more than a modest multiple of $\kappa(A) \times 10^{-6}$.
Table 5.5

\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline
\textbf{Method} & \textbf{iter} & \textbf{time} & \textbf{mv} & \textbf{iter} & \textbf{time} & \textbf{mv} & \textbf{iter} & \textbf{time} & \textbf{mv} \\
\hline
\textbf{IRRHLB} & 1116 & 263 & 30320 & 886 & 405 & 31900 & 947 & 918 & 43566 \\
\textbf{IRRLB} & n.c. & - & - & n.c. & - & - & 1604 & 1522 & 73788 \\
\hline
\textbf{IRRHLB} & 1520 & 496 & 36486 & 1139 & 761 & 38732 & 971 & 978 & 42730 \\
\hline
\textbf{IRRLB} & n.c. & - & - & n.c. & - & - & 1116 & 1113 & 49110 \\
\hline
\textbf{IRRHLB} & 1931 & 1906 & 81110 & 1656 & 2439 & 86120 & \\
\hline
\end{tabular}

We had more observations on the behavior of IRHLB, IRLB, IRLBA and IRLANB on these three difficult problems. For example, the residual norms obtained may oscillate but decrease very slowly; they may first decrease to some stage and then oscillate; they may have first decrease, then stabilize and do not decrease further; they may decrease to some stage and then increase. Therefore, IRRHLB is not only the best but also the unique choice for fidap4, jagmesh8 and lshp3025 for most of the given \(k\)'s and \(m\)'s.

We tested well1850, pde2961, dw2048 and plat1919 for \(\texttt{opts.tol} = 1e^{-6}, 1e^{-9}\), respectively. Tables 5.6–5.9 report the results for \(\texttt{opts.tol} = 1e^{-6}\). We do not list the corresponding results for \(\texttt{opts.tol} = 1e^{-9}\), as will be explained shortly.

We found that all the algorithms computed the desired smallest singular values correctly once they converged. The computed smallest singular values had relative errors no more than a very modest multiple of \(\kappa(A) \times 10^{-6}\). We observed that, in terms of restarts and matrix-vector products, IRRHLB was often considerably more efficient and several times faster than the others except IRRLB. IRRLB was nearly as efficient as IRRHLB in many cases, and it was slightly better than IRRHLB in a few cases; see, e.g., Table 5.7–5.8 for the results on dw2048 for \(m = 50\) and pde2961 for \(k = 1, 3, m = 50\). However, for the relatively difficult plat1919, it was less robust than IRRHLB and failed to converge for some \(k\) and \(m\); see Table 5.9. IRLB, IRLA and IRLANB were less robust and efficient than IRRLB, as the tables indicate. In addition, the results demonstrate that the bigger \(k\) was, the more restarts the algorithms used generally.

For \(\texttt{opts.tol} = 1e^{-9}\), we observed similar phenomena and had similar findings. The only essential exception is that for plat1919 and \(k = 5, m = 15\), IRRLB did not converge after 2000 restarts were used. Furthermore, we found that for the four test matrices all the algorithms used more restarts for \(\texttt{opts.tol} = 1e^{-9}\) than those for \(\texttt{opts.tol} = 1e^{-6}\) and they continued converging very smoothly from \(\texttt{opts.tol} = 1e^{-6}\) to \(\texttt{opts.tol} = 1e^{-9}\), provided they converged. Hence we do not list the results anymore.

To be more illustrative, we draw some typical curves that feature general convergence processes of the six algorithms. Figures 5.3–5.4 depict absolute residual norms versus restarts for well1850 when \(k = 1, 3\) and \(\texttt{opts.tol} = 1e^{-6}, 1e^{-9}\), respectively. The figures clearly demonstrate that IRRHLB is the fastest, IRRLB is the second best, IRHLB is faster than IRLB while IRHLB, IRLB, IRLA and IRLANB
are comparable and competitive though IRLANB may be slightly slower. The tables tell us that IRHLB was faster than IRLB. We see from the figures that after some stages the algorithms started converging quite smoothly and they used more but not too many more restarts for the smaller $\text{opts.tol} = 1e^{-9}$. Besides, for IRLANB, we see that they computed the smallest singular triplet after many restarts then found the second and third smallest singular triplets very quickly. This is because after the previous singular triplet(s) was (were) computed the available subspaces contained rich information on the later desired singular vectors.
Table 5.7

dw2048 for $k = 1, 3, 5, 10$, tol = $1e − 6$

| $m$ | Algorithms | $k = 1$ |  
|-----|------------|------|------|------|
|     |            | 30   | 40   | 50   |
|     |            | iter | time | mv   | iter | time | mv   | iter | time | mv   |
| IRRHLB | 93 | 24.8 | 2242 | ?? | 38.1 | 2776 | 64 | 37.7 | 2948 |
| IRRLB | 156 | 36.9 | 4060 | 52 | 23.3 | 1876 | 46 | 30.0 | 2120 |
| IRHLB | 236 | 59.6 | 6140 | 128 | 57.2 | 4612 | 82 | 47.9 | 3776 |
| IRLB  | 266 | 67.5 | 6920 | 154 | 62.9 | 5224 | 93 | 57.5 | 4282 |
| IRLBA | 276 | 9.71 | 7180 | 148 | 7.54 | 5332 | 89 | 6.64 | 3526 |
| IRLANB | 406 | 64.2 | 10155 | 142 | 70.0 | 7670 | 142 | 60.4 | 6395 |

| $m$ | Algorithms | $k = 3$ |  
|-----|------------|------|------|------|
|     |            | 30   | 40   | 50   |
|     |            | iter | time | mv   | iter | time | mv   | iter | time | mv   |
| IRRHLB | 100 | 22.7 | 2406 | 81 | 34.8 | 2760 | 67 | 40.9 | 2954 |
| IRRLB | 117 | 26.2 | 2814 | 72 | 31.5 | 2454 | 46 | 32.8 | 2030 |
| IRHLB | 209 | 40.8 | 5022 | 110 | 41.8 | 3746 | 71 | 42.7 | 3130 |
| IRLB | 230 | 44.0 | 5526 | 120 | 45.2 | 4086 | 78 | 44.9 | 3438 |
| IRLBA | 238 | 7.84 | 5718 | 124 | 6.21 | 4222 | 80 | 5.55 | 3526 |
| IRLANB | 280 | 29.3 | 6447 | 142 | 42.7 | 4693 | 92 | 35.5 | 3963 |

| $m$ | Algorithms | $k = 5$ |  
|-----|------------|------|------|------|
|     |            | 30   | 40   | 50   |
|     |            | iter | time | mv   | iter | time | mv   | iter | time | mv   |
| IRRHLB | 107 | 22.6 | 2362 | 80 | 30.9 | 2568 | 69 | 49.8 | 2906 |
| IRRLB | 146 | 32.7 | 6220 | 75 | 35.2 | 2408 | 49 | 33.6 | 2066 |
| IRHLB | 186 | 31.5 | 4100 | 95 | 32.7 | 3048 | 63 | 35.1 | 2654 |
| IRLB | 266 | 47.0 | 5860 | 134 | 43.0 | 4296 | 85 | 47.8 | 3578 |
| IRLBA | 287 | 9.27 | 6321 | 142 | 6.79 | 4552 | 89 | 6.06 | 3746 |
| IRLANB | 224 | 28.9 | 4713 | 114 | 23.4 | 3543 | 73 | 28.0 | 3002 |

| $m$ | Algorithms | $k = 10$ |  
|-----|------------|------|------|------|
|     |            | 30   | 40   | 50   |
|     |            | iter | time | mv   | iter | time | mv   | iter | time | mv   |
| IRRHLB | 190 | 38.9 | 3243 | 110 | 46.2 | 2983 | 89 | 67.7 | 3306 |
| IRRLB | 246 | 51.4 | 4195 | 136 | 65.2 | 3685 | 68 | 54.1 | 2529 |
| IRHLB | 443 | 63.5 | 7544 | 187 | 59.3 | 5062 | 110 | 56.8 | 4083 |
| IRLB | 483 | 69.0 | 8224 | 203 | 63.6 | 5494 | 117 | 60.0 | 4342 |
| IRLBA | 335 | 9.99 | 5636 | 159 | 7.21 | 4250 | 90 | 5.85 | 3322 |
| IRLANB | 546 | 54.7 | 8750 | 222 | 43.7 | 5786 | 126 | 44.2 | 4550 |

We have done more experiments and have similar findings. Based on them, we may conclude that IRRHLB is the best and the most robust for general purpose and IRRLB is the second best. As far as overall efficiency is concerned, in terms of restarts and matrix-vector products, IRRHLB is the fastest and IRRLB is the second best while IRHLB, IRLB, IRLBA and IRLANB are all comparable each other and no one is considerably superior to the others. A further observation tells us that IRHLB is faster than IRLB. That IRRHLB is superior to IRRLB and IRHLB is better than IRLB sheds light on the fact argued in the introduction: The refined harmonic
Table 5.8
\( pde2961 \) for \( k = 1, 3, 5, 10, \) tol = \( 1 \epsilon - 6 \)

\[
\begin{array}{|c|c|c|c|c|c|c|c|}
\hline
m & \multicolumn{3}{|c|}{k = 1} & \multicolumn{3}{|c|}{k = 3} & \multicolumn{3}{|c|}{k = 5} & \multicolumn{3}{|c|}{k = 10} \\
\hline
\text{Algorithms} & \text{iter} & \text{time} & \text{mv} & \text{iter} & \text{time} & \text{mv} & \text{iter} & \text{time} & \text{mv} & \text{iter} & \text{time} & \text{mv} \\
\hline
\text{IRRHLB} & 127 & 44.1 & 3306 & 113 & 62.2 & 3848 & 101 & 83.1 & 4450 & 127 & 80.7 & 4765 \\
\text{IRRLB} & 230 & 77.7 & 5984 & 149 & 90.3 & 5072 & 85 & 63.3 & 3746 & 149 & 90.3 & 5072 \\
\text{IRHLB} & 371 & 116 & 9650 & 239 & 131 & 8132 & 146 & 113 & 6430 & 239 & 131 & 8132 \\
\text{IRLB} & 425 & 136 & 11054 & 272 & 134 & 9254 & 167 & 139 & 7354 & 272 & 134 & 9254 \\
\text{IRLBA} & 463 & 21.6 & 12042 & 284 & 19.3 & 9662 & 172 & 16.3 & 7574 & 284 & 19.3 & 9662 \\
\text{IRLANB} & 490 & 100 & 12255 & 339 & 111 & 11194 & 204 & 97.3 & 8779 & 339 & 111 & 11194 \\
\hline
\end{array}
\]

projection and the harmonic projection are more suitable for computing the smallest singular triplets than the refined standard projection and the standard projection, respectively. Meanwhile, we find that, as far as CPU timings are concerned, IRRHLB can be inferior to IRLBA. This may be partly because \( A \) is not very large or \( A \) too sparse, so that the savings of the first \( k + 3 \) steps of the Lanczos bidiagonalization process cannot compensate implicit restarting with \( m - (k + 3) \) shifts, and partly because our code for implicit restarting is far from optimized. In any event, as a whole, we can draw an overall conclusion that IRRHLB is at least competitive with
and can be much more efficient than the five other state of the art algorithms in both robustness and efficiency.

The advantages of IRRHLB are twofold: It extracts the best left and right approximate singular vectors from the given subspaces in the sense of residual minimizations; it uses the better refined harmonic shifts to construct better subspaces at each restart. Each of these two advantages alone may not gain much. However, as restarts proceed, the cumulative effect of their combination may be very striking, making IRRHLB much more efficient than the other algorithms. Similar comments

### Table 5.9

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and can be much more efficient than the five other state of the art algorithms in both robustness and efficiency.
A REFINED HARMONIC LANCZOS BIDIAGONALIZATION METHOD

Fig. 5.3. Convergence curves of well1850 with \( k = 1 \) and tol = 1e−6, 1e−9.

are made on the refined algorithms for the large eigenproblem in [15, 17].

6. Concluding remarks. We have presented the refined harmonic Lanczos bidiagonalization method for computing the smallest singular triplets of large matrices. We have developed a practical implicitly restarted algorithm with the refined harmonic shifts scheme suggested. We have done many numerical experiments and have compared the new algorithm with five other state of the art algorithms. The results show that the new algorithm is at least competitive with and can be much more efficient than the five other algorithms in both robustness and efficiency.

We have reported the numerical results of computation of the smallest singular triplets. We have also done many numerical experiments on computation of the largest singular triplets. As indicated in [20], IRRLB is generally preferable to IRLB [20, 23], PROPACK [24], LANSO [23, 24] and svds as well as some others; it is the most robust among the restarted algorithms. Note that IRLANB is designed to only compute the smallest singular triplets. For computation of the largest singular triplets, we have found that IRRLB is at least competitive with the four other algorithms, in which IRLBA uses Ritz approximations. However, more observations reveal that IRRHLB and IRHLB are considerably inferior to IRRLB and IRLB, respectively. This suggests that IRRHLB and IRHLB are suitable for computing both the largest singular triplets and the smallest ones but IRRHLB and IRHLB are more suitable for computing the smallest singular triplets.

The Matlab codes of IRRHLB, IRRLB, IRHLB and IRLB can be obtained from
Fig. 5.4. Convergence curves of well1850 with $k = 3$ and $\text{tol} = 1e^{-6}, 1e^{-9}$.

Acknowledgements. We thank two referees very much for their very valuable and helpful suggestions and comments, which made us improve on the presentation considerably. Many thanks also go to Kokiopoulou, Bekas, Gallopoulos and Baglama and Reichel for generously providing us their IRLANB and IRLBA codes, which made our numerical experiments and comparisons possible.

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