THE JOINT BIDIAGONALIZATION METHOD FOR LARGE GSVD COMPUTATIONS IN FINITE PRECISION

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Abstract. The joint bidiagonalization (JBD) method has been used to compute some extreme generalized singular values and vectors of a large regular matrix pair \(\{A, L\}\), where we propose three approaches to compute approximate generalized singular values and vectors. We make a numerical analysis of the underlying JBD process and establish relationships between it and two mathematically equivalent Lanczos bidiagonalizations in finite precision. Based on the results of numerical analysis, we investigate the convergence of the approximate generalized singular values and vectors of \(\{A, L\}\). The results show that, under some mild conditions, the semiorthogonality of Lanczos type vectors suffices to deliver approximate generalized singular values with the same accuracy as the full orthogonality does, meaning that it is only necessary to seek for efficient semiorthogonalization strategies for the JBD process. We also establish a sharp bound for the residual norm of an approximate generalized singular value and corresponding approximate right generalized singular vectors, which can reliably estimate the residual norm without explicitly computing the approximate right generalized singular vectors before the convergence occurs.

Key words. generalized singular value decomposition, joint bidiagonalization, Lanczos bidiagonalization, rounding error, orthogonality level, Ritz value, reorthogonalization, residual norm

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1. Introduction. In [37], Zha presents a joint bidiagonalization (JBD) process that jointly bidiagonalizes a large sparse or structured matrix pair \(\{A, L\}\) to upper diagonal forms successively, where \(A \in \mathbb{R}^{m \times n}\) and \(L \in \mathbb{R}^{p \times n}\). He exploits the JBD process to compute a few extreme generalized singular values and vectors of \(\{A, L\}\) [25, 35, 36]. Kilmer et al. [16] develop a variant of the JBD process that jointly reduces \(\{A, L\}\) to lower and upper bidiagonal forms simultaneously. Besides the computation of a few extreme generalized singular value decomposition (GSVD) components, this variant is used to solve large scale linear discrete ill-posed problems with general-form regularization, where \(L\) is the regularization matrix [6, 7, 15, 16].

The JBD process of \(\{A, L\}\) is mathematically equivalent to Lanczos bidiagonalizations [2, 5, 26] of two certain related matrices, as we will describe next. Consider the compact QR factorization of the stacked matrix:

\[
\begin{pmatrix}
A \\
L
\end{pmatrix} = QR = \begin{pmatrix}
Q_A \\
Q_L
\end{pmatrix} R,
\]

where \(Q \in \mathbb{R}^{(m+p) \times n}\) is column orthonormal and \(R \in \mathbb{R}^{n \times n}\) is upper triangular, and \(Q_A \in \mathbb{R}^{m \times n}\) and \(Q_L \in \mathbb{R}^{p \times n}\). If \(\text{rank}(A^T L^T) = n\) with \(\text{rank}(\cdot)\) the rank of a matrix, we call the pair \(\{A, L\}\) is regular; in this case, \(R\) is nonsingular.

Applying the BIDIAG-1 algorithm and the BIDIAG-2 algorithm in [26], which are the lower and upper Lanczos bidiagonalizations, to \(Q_A\) and \(Q_L\), respectively, we
can reduce $Q_A$ and $Q_L$ to the following lower and upper bidiagonal matrices:

$$B_k = \begin{pmatrix} \alpha_1 & \beta_2 & \alpha_2 & \cdots \\ \beta_3 & \alpha_3 & \ddots & \cdots \\ \vdots & \ddots & \ddots & \alpha_k \\ \beta_k & \cdots & \alpha_k & \beta_{k+1} \end{pmatrix} \in \mathbb{R}^{(k+1) \times k}, \quad \hat{B}_k = \begin{pmatrix} \hat{\alpha}_1 & \hat{\beta}_2 & \cdots \cdots \cdots \\ \hat{\alpha}_2 & \cdots & \cdots & \hat{\beta}_{k-1} \\ \vdots & \ddots & \ddots & \vdots \\ \hat{\alpha}_k & \cdots & \cdots & \hat{\beta}_k \end{pmatrix} \in \mathbb{R}^{k \times k}.$$ 

The above two algorithms produce the four orthonormal matrices

$$U_{k+1} = (u_1, \ldots, u_{k+1}) \in \mathbb{R}^{m \times (k+1)}, \quad V_k = (v_1, \ldots, v_k) \in \mathbb{R}^{n \times k}$$

and

$$\hat{U}_k = (\hat{u}_1, \ldots, \hat{u}_k) \in \mathbb{R}^{p \times k}, \quad \hat{V}_k = (\hat{v}_1, \ldots, \hat{v}_k) \in \mathbb{R}^{n \times k}.$$ 

The BIDIAG-1 and BIDIAG-2 algorithms can be related by taking the starting vector $\hat{v}_1 = v_1$ in BIDIAG-2. It has been proved in [16, 37] that the Lanczos vectors $\hat{v}_i$ and the elements $\hat{\alpha}_i, \hat{\beta}_i$ of $\hat{B}_k$ have the following relations:

$$\hat{v}_{i+1} = (-1)^i v_{i+1}, \quad \hat{\beta}_i = \alpha_{i+1} / \hat{\alpha}_i.$$ 

For $A$ and $L$ large, the explicit QR factorization (1.1) is generally impractical due to the excessive storage and/or computational cost. It can be avoided by solving a least squares problem with $(AT, L^T)T$ as the coefficient matrix at each iteration $i, i = 1, 2, \ldots, k$. Zha [37] and Kilmer, Hansen and Espanol [16] propose the JBD process that successively reduces $\{A, L\}$ to $\{B_k, \hat{B}_k\}$, where $\hat{B}_k = B_k D_k$ with $D_k = \text{diag}(1, -1, \ldots, (-1)^{k-1}) \in \mathbb{R}^{k \times k}$, which will be described in the next section. The $k$-step JBD process explicitly computes three orthonormal matrices $U_{k+1} \in \mathbb{R}^{m \times (k+1)}$, $\hat{U}_k \in \mathbb{R}^{p \times k}$, and $\hat{V}_k \in \mathbb{R}^{(m+n) \times k}$ and the lower and upper bidiagonal matrices $B_k$ and $\hat{B}_k$. The matrices $V_k$ and $\hat{V}_k$ in the BIDIAG-1 and BIDIAG-2 algorithms are related to $V_k$ by $V_k = Q^T \hat{V}_k$ and $\hat{V}_k = V_k D_k$. Therefore, the JBD process on $\{A, L\}$ is mathematically equivalent to the joint lower and upper Lanczos bidiagonalizations of $Q_A$ and $Q_L$, when taking $\hat{v}_1 = v_1$. 

The lower bidiagonal $B_k$ is the Ritz–Galerkin projection of $Q_A$ on the left subspace span$(U_{k+1})$ and the right subspace span$(V_k)$, while the upper bidiagonal $\hat{B}_k$ is the Ritz–Galerkin projection of $Q_L$ on the left and right subspaces span$(\hat{U}_k)$ and span$(\hat{V}_k)$, where span$(\cdot)$ denotes the subspace spanned by the columns of a matrix. Therefore, the extreme singular values of $Q_A$ or $Q_L$ can be approximated by those of $B_k$ or $\hat{B}_k$, and the extreme generalized singular values of $\{A, L\}$ can be approximated by those of $\{B_k, \hat{B}_k\}$ since the generalized singular values of $\{A, L\}$ are identical to those of $\{Q_A, Q_L\}$ [15, 37]. 

Due to the influence of rounding errors, we have numerically observed that the orthogonality of the three sets of basis vectors, also called Lanczos vectors conventionally, computed by the JBD process loses gradually. This is a typical phenomenon in Lanczos type algorithms, such as the symmetric Lanczos process [17] and the Lanczos bidiagonalization process [18]. The loss of orthogonality of Lanczos vectors leads to a delay of convergence of some extreme eigenvalues and the appearance of spurious computed Ritz values, i.e., ghost Ritz values, [20, 21, 22, 24]. To fix this deficiency, several reorthogonalization strategies have been proposed to maintain some level of
orthogonality of the computed Lanczos vectors in order to ensure the convergence of the computed Ritz values [28, 30, 31]. Particularly, Simon [30] proves that the semiorthogonality of Lanczos vectors suffices to guarantee that the computed Ritz values have the same accuracy as the full orthogonality does and avoid spurious computed Ritz values. The above results on the symmetric Lanczos process have been extended by Larsen [18] to Lanczos bidiagonalization, based on which he proposes an efficient partial reorthogonalization strategy. Later on, Simon and Zha in [32] propose a one-sided reorthogonalization strategy on the computed right Lanczos vectors. Barlow [1] makes a backward error analysis of the one-sided reorthogonalization scheme and proves that Lanczos bidiagonalization applied to a matrix $C$ in finite precision produces Krylov subspaces generated by a nearby matrix $C + E$, where $E$ is an error matrix depending on the orthogonality level of the computed right Lanczos vectors.

Denote the unit roundoff by $\epsilon$. In the presence of rounding errors, among many others, a central concern is whether or not the JBD process for computing $U_{k+1}$, $V_k$ and $B_k$ is equivalent to the standard lower Lanczos bidiagonalization of $Q_A$ with the rounding error $O(\epsilon)$ and whether or not the process for computing $\hat{U}_k$, $\hat{V}_k$ and $\hat{B}_k$ is equivalent to the upper Lanczos bidiagonalization of $Q_L$ with the rounding error $O(\epsilon)$. There has been yet no result on the finite precision behavior of the JBD process. In this paper, we will focus on it and, based on some underlying round-off error models and results, make a numerical analysis of the JBD process. We will derive a number of properties of the JBD process in finite precision. Our contributions mainly consist of the following three parts.

First, we will show that the equivalence of the JBD process and standard lower and upper Lanczos bidiagonalizations does not hold in finite precision unconditionally. That is, the finite precision forms resulting from the JBD process may be no longer the corresponding ones of standard Lanczos bidiagonalizations if there are no additional conditions. We will investigate what a role rounding errors play in the loss of this equivalence and in what way rounding errors are amplified.

Second, in finite precision, we will show that the orthogonality levels of $U_{k+1}$, $\tilde{V}_k$ and $\tilde{U}_k$ are closely related and those of $\tilde{V}_k$ and $\tilde{V}_k$ interact too. In particular, we derive an upper bound for the orthogonality level of $\tilde{U}_k$, which is shown to be controlled by not only the orthogonality levels of $\tilde{V}_k$ and $U_{k+1}$ but also a gradually growing quantity $\|\tilde{B}_k^{-1}\|$. The result indicates that the orthogonality level of $\tilde{U}_k$ is similar to those of $U_{k+1}$ and $\tilde{V}_k$, provided that $\tilde{B}_k$ is not ill conditioned. Therefore, when designing a reorthogonalization strategy for the JBD process, one reorthogonalizes only $u_i$ and $\tilde{v}_i$ but $\tilde{u}_i$, which can save considerable reorthogonalization work.

Third, we shall show how to make use of the JBD process to compute extreme GSVD components of $\{A, L\}$, leading to the JBD method for the large GSVD computation. Precisely, we will propose three approaches to compute approximate generalized singular values and approximate right generalized singular vectors by exploiting the SVDs of $B_k$ and $\tilde{B}_k$ and the GSVD of $\{B_k, \tilde{B}_k\}$, respectively; we will present two approaches to compute approximate left generalized singular vectors of $A$ and $L$ via either the left singular vectors of $B_k$ and $\tilde{B}_k$ simultaneously or the left generalized singular vectors of $\{B_k, \tilde{B}_k\}$. We will investigate the convergence of the approximate generalized singular values that are computed by the singular values of $B_k$ or $\tilde{B}_k$. Similarly to Lanczos bidiagonalization, the loss of orthogonality of Lanczos type vectors computed by the JBD process leads to a delay of the convergence of the computed Ritz values and the appearance of spurious copies. We show that, under the assumptions that $\|B_k^{-1}\|$ and $\|\tilde{B}_k^{-1}\|$ are modest uniformly with $k$, the semiorthogo-
nality of Lanczos type vectors suffices to avoid spurious copies and guarantees that the approximate generalized singular values have the same accuracy as the full orthogonality does. Here the semiorthogonality means that the absolute value of inner product of two unit length vectors is at the level of $O(\epsilon^{1/2})$, in contrast to the full orthogonality level $O(\epsilon)$. Therefore, the semiorthogonality of Lanczos vectors suffices for the JBD method. In the meantime, we study the residual norm of an approximate generalized singular value and approximate right generalized singular vector, whose size is used to design a stopping tolerance for the JBD method. In finite precision, we derive an upper bound for the residual norm, and show that this upper bound can replace the residual norm to design a reliable stopping criterion without explicitly computing approximate right generalized singular vectors before the convergence occurs. We only compute the approximate right generalized singular vectors by solving certain consistent least squares problems with the coefficient matrix $(A^T, L^T)^T$ at the convergence rather than doing so at each iteration.

The paper is organized as follows. In Section 2, we review the GSVD of $\{A, L\}$ and describe the JBD process in exact arithmetic. In Section 3, we make a numerical analysis of the JBD process in finite precision. We establish relationships between the JBD process and two lower and upper Lanczos bidiagonalizations, and investigate interactions of orthogonality levels of the computed Lanczos type vectors. In Section 4, we describe the JBD method for computing a number of extreme generalized singular values and vectors of $\{A, L\}$, and discuss the convergence and stopping criteria. In Section 5, we report numerical experiments to confirm our results. Finally, we conclude the paper with some remarks and future work in Section 6.

Throughout the paper, we denote by $I_k$ the identity matrix of order $k$, by $0_k$ and $0_{k \times l}$ the $k$-dimensional zero vector and the $k \times l$ zero matrix, respectively. The transpose of a matrix $C$ is denoted by $C^T$, and $\| \cdot \|$ is the 2-norm of a matrix.

2. GSVD and the JBD process. We describe the GSVD of $\{A, L\}$ and the JBD process with some of its basic properties. Let the compact QR factorization of $(A^T, L^T)^T$ be defined as (1.1) and

\[ QA = P_A C_A W^T, \quad Q_L = P_L S_L W^T \]

be the CS decomposition of the matrix pair $\{Q_A, Q_L\}$ [5, §2.5.4], where $P_A \in \mathbb{R}^{m \times m}$, $P_L \in \mathbb{R}^{p \times p}$ and $W \in \mathbb{R}^{n \times n}$ are diagonal matrices (not necessarily orthogonal matrices), and $C_A \in \mathbb{R}^{m \times n}$ and $S_L \in \mathbb{R}^{p \times n}$ are orthogonal matrices, and the generalized

Suppose that rank$((A^T, L^T)^T) = r$. It is shown in [25] that $C_A$ and $S_L$ can be written as

\[ C_A = \begin{pmatrix} \Sigma_A & 0 \\ r & n-r \end{pmatrix} \]

\[ S_L = \begin{pmatrix} \Sigma_L & 0 \\ r & n-r \end{pmatrix} \]

where

\[ \Sigma_A = \begin{pmatrix} I_q & C_l \\ C_l & O \end{pmatrix} \]

\[ \Sigma_L = \begin{pmatrix} O & S_l \\ S_l & I_l \end{pmatrix} \]

Write $C_l = \text{diag}(c_{q+1}, \ldots, c_{q+l})$, $c_{q+1} \geq \cdots \geq c_{q+l} > 0$ and $S_l = \text{diag}(s_{q+1}, \ldots, s_{q+l})$, $0 < s_{q+1} \leq \cdots \leq s_{q+l}$. Then $c_i^2 + s_i^2 = 1$, $i = q+1, \ldots, q+l$, and the generalized
singular values of \( \{A, L\} \) are

\[
\underbrace{0, \ldots, 0}_{t}, \quad \underbrace{c_{q+1}/s_{q+1}, \ldots, c_{q+1}/s_{q+1}}_{l}, \quad \underbrace{t-\infty, \ldots, \infty}_{q}
\]

where \( t = r - q - l \).

To ease the presentation, in the sequel, we always assume that \( \{A, L\} \) is regular. Then \( R \) in (1.1) is nonsingular and the GSVD of \( \{A, L\} \) is

\[
A = P_A C_A X^{-1}, \quad L = P_L S_L X^{-1}
\]

with \( X = R^{-1} W \in \mathbb{R}^{n \times n} \). Let \( X = (x_1, \ldots, x_n) \), \( P_A = (p_A^1, \ldots, p_A^n) \) and \( P_L = (p_L^1, \ldots, p_L^p) \). We can write the GSVD (2.2) in the vector form:

\[
\begin{align*}
Ax_i &= c_i p_A^i, \\
Lx_i &= s_i p_L^i, \\
s_i A^T p_A^i &= c_i L^T p_L^i,
\end{align*}
\]

where the \( i \)-th large generalized singular value of \( \{A, L\} \) is \( c_i/s_i \), and the \( i \)-th corresponding generalized singular vectors are \( x_i, p_A^i \) and \( p_L^i \), respectively. We call \( x_i \) the right generalized singular vector, \( p_A^i \) and \( p_L^i \) the left generalized singular vectors corresponding to \( c_i/s_i \). Since \( c_i/s_i = \infty \) and \( c_i/s_i = 0 \) when \( s_i = 0 \) and \( s_i = 1 \), it is more convenient to use pair \( \{c_i, s_i\} \) to denote \( c_i/s_i \). We also note that each \( x_i \) satisfies the normalization \( x_i^T (A^T A + L^T L) x_i = 1 \).

We describe the JBD process [16] as Algorithm 1, which, in exact arithmetic, corresponds to the lower and upper Lanczos bidiagonalization of \( Q_A \) and \( Q_L \), respectively:

\[
\begin{align*}
Q_A V_k &= U_{k+1} B_k, \quad Q_A^T U_{k+1} = V_k B_k^T + \alpha_{k+1} v_{k+1} e_{k+1}^T, \\
Q_L \hat{V}_k &= \hat{U}_k \hat{B}_k, \quad Q_L^T \hat{U}_k = \hat{V}_k \hat{B}_k^T + \hat{\beta}_k \hat{v}_{k+1} e_{k+1}^T
\end{align*}
\]

with \( \hat{v}_1 = v_1 \), where \( e_k \) is the last column of \( I_k \), which are \( k \)-step lower and upper Lanczos bidiagonalization processes of \( Q_A \) and \( Q_L \), respectively.

**Algorithm 1** The \( k \)-step JBD process

1. Choose a nonzero starting vector \( b \in \mathbb{R}^m \), and let \( \beta_1 u_1 = b, \beta_1 = \|b\| \)
2. \( \alpha_1 \hat{v}_1 = QQ^T \begin{pmatrix} u_1 \\ 0_p \end{pmatrix} \)
3. \( \hat{\alpha}_1 \hat{u}_1 = \hat{v}_1 (m + 1 : m + p) \)
4. for \( i = 1, 2, \ldots, k \), do
5. \( \beta_{i+1} u_{i+1} = \hat{v}_i (1 : m) - \alpha_i u_i \)
6. \( \alpha_{i+1} \hat{v}_{i+1} = QQ^T \begin{pmatrix} u_{i+1} \\ 0_p \end{pmatrix} - \beta_{i+1} \hat{v}_i \)
7. \( \hat{\beta}_i = (\alpha_{i+1} \beta_{i+1})/\hat{\alpha}_i \)
8. \( \hat{\alpha}_{i+1} u_{i+1} = (-1)^i \hat{v}_{i+1} (m + 1 : m + p) - \hat{\beta}_i \hat{u}_i \)
9. end for

At each iteration \( i = 1, 2, \ldots, k \), Algorithm 1 needs to compute \( QQ^T \begin{pmatrix} u_i \\ 0_p \end{pmatrix} \). For \( A \) and \( L \) large, however, the compact QR factorization (1.1) of \( (A^T, L^T)^T \) is generally
impractical, that is, both $Q$ and $R$ are not available. Let $\hat{u}_i = \begin{pmatrix} u_i \\ 0_p \end{pmatrix}$. Since $QQ^T \hat{u}_i$ is nothing but the orthogonal projection of $\hat{u}_i$ onto the column space of $(A^T, L^T)^T$, we have $QQ^T \hat{u}_i = \begin{pmatrix} A \\ L \end{pmatrix} \hat{x}_i$, where
\begin{equation}
\hat{x}_i = \arg \min_{\hat{x} \in \mathbb{R}^n} \left\| \begin{pmatrix} A \\ L \end{pmatrix} \hat{x} - \hat{u}_i \right\|.
\end{equation}

This large scale least squares problem can be solved by an iterative solver, e.g., the most commonly used LSQR algorithm [26].

In exact arithmetic, the $k$-step JBD process produces the two bidiagonal matrices $B_k$, $\bar{B}_k$ and three orthonormal matrices $U_{k+1}$, $\bar{U}_k$ in (1.3)–(1.4) and
\begin{equation}
\tilde{V}_k = (\tilde{v}_1, \ldots, \tilde{v}_k) \in \mathbb{R}^{(m+p) \times k},
\end{equation}
where $\tilde{v}_i = Qv_i$ with $v_i$ the $i$-th column of $V_k$ in (1.3), i.e., $v_i = Q^T \tilde{v}_i$. It can be written as
\begin{align}
(I_m, 0_{m \times p}) \tilde{V}_k &= U_{k+1} B_k, \\
QQ^T \begin{pmatrix} U_{k+1} \\ 0_{p \times (k+1)} \end{pmatrix} &= \tilde{V}_k B_k^T + \alpha_{k+1} \tilde{v}_{k+1} e_{k+1}^T, \\
(0_{p \times m}, I_p) \tilde{V}_k D_k &= \bar{U}_k \bar{B}_k,
\end{align}
where $D_k = \text{diag}(1, -1, \ldots, (-1)^{k-1}) \in \mathbb{R}^{k \times k}$, and $e_{k+1}$ is the last column of $I_{k+1}$.

It is shown [16] that, in exact arithmetic, the $k$-step JBD process satisfies
\begin{equation}
AZ_k = U_{k+1} B_k, \quad LZ_k = \bar{U}_k \bar{B}_k,
\end{equation}
where $Z_k = R^{-1} V_k = (z_1, \ldots, z_k)$ and $\bar{B}_k = \bar{B}_k D_k$, and
\begin{equation}
B_k^T B_k + \bar{B}_k^T \bar{B}_k = I_k.
\end{equation}
Therefore, the singular values of $B_k$ are determined by those of $\bar{B}_k$, i.e., $\bar{B}_k$, and vice versa. As a result, if some extreme generalized singular values of $\{A, L\}$ are of interest, one can use the extreme generalized singular values of $\{B_k, \bar{B}_k\}$ to approximate them by either computing the generalized singular values of the small pairs or only computing the singular values of $B_k$ or $\bar{B}_k$.

In finite precision, it is well known that the Lanczos vectors computed by Lanczos bidiagonalization gradually lose their mutual orthogonality as the iteration number $k$ increases [18]. Following [18, 32], we define the orthogonality level of a set of vectors as follows.

**Definition 2.1.** For a rectangular matrix $W_k = (w_1, \ldots, w_k) \in \mathbb{R}^{r \times k}$ with $\|w_j\| = 1$, $j = 1, \ldots, k$, we call $\xi^w_{ij} = w_i^T w_j$ the orthogonality level among $w_i$ and $w_j$. The orthogonality level of $\{w_1, \ldots, w_k\}$ or $W_k$ is measured by one of
\begin{align}
\xi(W_k) &= \max_{1 \leq i \neq j \leq k} \xi^w_{ij}, \\
\eta(W_k) &= \|I_k - W_k^T W_k\|.
\end{align}
Notice that \( \xi(W_k) \leq \eta(W_k) \leq k \xi(W_k) \). The above two quantities can be used interchangeably to measure the orthogonality level of Lanczos vectors. Let \( \sigma_i(\cdot) \) and \( \lambda_i(\cdot) \) be the \( i \)-th largest singular value and eigenvalue of a symmetric matrix respectively. Then

\[
\sigma_i^2(W_k) = \lambda_i(W_k^TW_k) = 1 + \lambda_i(W_k^TW_k - I_k) \leq 1 + \| I_k - W_k^TW_k \|,
\]

which leads to

\[
\| W_k \| \leq \sqrt{1 + \eta(W_k)}.
\]

For Lanczos bidiagonalization, the loss of orthogonality of the Lanczos vectors will lead to appearance of spurious Ritz values and a delay of the convergence of \( \| \cdot \| \). From now on, without confusion, we use the same notation as before to denote computation, and grasp essential features but discard those irrelevant or negligible.

3. The JBD process in finite precision. When it is carried out in finite precision, due to the influence of rounding errors, the behavior of the JBD process will deviate from that in exact arithmetic. First, the JBD process of \( \{A, L\} \) is not equivalent to the combination of the two Lanczos bidiagonalizations any longer. Second, the three matrices \( U_{k+1}, V_k \) and \( U_k \) lose their numerical orthogonality gradually as \( k \) increases. In this paper, we do not consider the solution accuracy of the inner least squares problem (2.6) at each iteration, though it has an important influence on the accuracy and efficiency of the algorithm. This issue is complicated, and we will study it in our future work. In the following analysis, we always assume that (2.6) is solved accurately, i.e., \( \begin{pmatrix} A \\ L \end{pmatrix} \) \( \hat{x}_i = Q Q^T \begin{pmatrix} u_i \\ 0_p \end{pmatrix} \).

First of all, we state a set of basics and assumptions on the behavior of the rounding errors occurring in the JBD process. They are adapted from the symmetric Lanczos process and Lanczos bidiagonalization, constitute a model for the actual computation, and grasp essential features but discard those irrelevant or negligible ones. From now on, without confusion, we use the same notation as before to denote the computed ones in finite precision. In this case, relations (2.8)–(2.10) add rounding error terms (cf. [27, §13.4]) and become

\[
(I_m, 0_{m \times p}) \tilde{V}_k = U_{k+1} B_k + \bar{F}_k, \tag{3.1}
\]

\[
Q Q^T \begin{pmatrix} U_{k+1} \\ 0_{p \times (k+1)} \end{pmatrix} = \tilde{V}_k B_k^T + \alpha_{k+1} \tilde{v}_{k+1} \tilde{e}_{k+1}^T + \bar{G}_{k+1}, \tag{3.2}
\]

\[
(0_{p \times m}, I_p) \tilde{V}_k D_k = \tilde{U}_k \bar{B}_k + \bar{F}_k, \tag{3.3}
\]

where the rounding error matrices \( \tilde{F}_k = (\tilde{f}_1, \ldots, \tilde{f}_k) \), \( \bar{G}_{k+1} = (\bar{g}_1, \ldots, \bar{g}_{k+1}) \) and \( \bar{F}_k = (\bar{f}_1, \ldots, \bar{f}_k) \) satisfy

\[
\| \bar{F}_k \|, \| \bar{G}_{k+1} \|, \| \bar{F}_k \| = O(\epsilon). \tag{3.4}
\]

Second, the following local orthogonality of \( u_i \) and \( \hat{u}_i \) holds [23, 30]:

\[
\beta_{i+1} | \hat{u}_{i+1}^T u_i | = O(c_1(m, n)\epsilon), \tag{3.5}
\]

\[
\hat{\alpha}_{i+1} | \hat{u}_{i+1}^T \hat{u}_i | = O(c_2(p, n)\epsilon), \tag{3.6}
\]
where \(c_1(m, n)\) and \(c_2(p, n)\) are modest constants depending on \(m, n\) and \(p\). Third, we assume that

\[
(3.7) \quad \text{neither } \beta_{i+1} \text{ nor } \hat{\alpha}_{i+1} \text{ ever becomes negligible,}
\]

which is almost always true in practice. In case either \(\beta_{i+1}\) or \(\hat{\alpha}_{i+1}\) becomes negligible, the JBD process should be terminated since it has found either acceptable approximate right invariant generalized singular subspace and left generalized singular subspace for \(A\) or acceptable approximate right invariant generalized singular subspace and left generalized singular subspace for \(L\), as can be justified from (2.4), (2.5) and (2.11). This can also be seen from the later Theorem 4.3 and \(\hat{\alpha}_i \hat{\beta}_i = \alpha_{i+1} \beta_{i+1}\) in step 7 of Algorithm 1. Finally, for simplicity, in our numerical analysis, we always assume that the computed Lanczos type vectors are of unit length.

### 3.1. Relationships between the JBD process and Lanczos bidiagonalization in finite precision

We show that, in finite precision, the JBD process of \(\{A, L\}\) is no longer equivalent to the combination of the lower and upper Lanczos bidiagonalizations of \(Q_A\) and \(Q_L\). To this end, we first present the following lemma.

**Lemma 3.1.** Let \(v_i = Q^T \tilde{v}_i, V_k = (v_1, \ldots, v_k)\) and \(\tilde{B}_k = \begin{pmatrix} B_k^T \\ \hat{\alpha}_k \tilde{C}_k \end{pmatrix} \in \mathbb{R}^{k \times k}\). Then

\[
(3.8) \quad \|\tilde{V}_k - QV_k\| \leq \|\tilde{G}_k \tilde{B}_k^{-1}\| = O(\|\tilde{B}_k^{-1}\| \epsilon)
\]

with \(\tilde{G}_k\) defined in (3.2).

**Proof.** Write the matrix \(C = (A^T, L^T)^T\). Then

\[
QQ^T = CC^\dagger, \quad QQ^T C = C, \quad QQ^T \begin{pmatrix} U_k \\ 0_{p \times k} \end{pmatrix} = CX_k,
\]

where “\(\dagger\)” denotes the Moore–Penrose inverse of a matrix and \(X_k = C^\dagger \begin{pmatrix} U_k \\ 0_{p \times k} \end{pmatrix}\). From (3.2) and \(V_k = Q^T \tilde{V}_k\), we have \(CX_k = \tilde{V}_k \tilde{B}_k + \tilde{G}_k\), leading to \(\tilde{V}_k = CX_k \tilde{B}_k^{-1} - \tilde{G}_k \tilde{B}_k^{-1}\). Therefore, we obtain

\[
(3.9) \quad \tilde{V}_k - QV_k = \tilde{V}_k - QQ^T \tilde{V}_k = \tilde{V}_k - QQ^T (CX_k \tilde{B}_k^{-1} - \tilde{G}_k \tilde{B}_k^{-1}) = \tilde{V}_k - CX_k \tilde{B}_k^{-1} + QQ^T \tilde{G}_k \tilde{B}_k^{-1} = -\tilde{G}_k \tilde{B}_k^{-1} + QQ^T \tilde{G}_k \tilde{B}_k^{-1} = (QQ^T - I_{m+p}) \tilde{G}_k \tilde{B}_k^{-1}.
\]

Taking norms in both sides proves (3.8). □

This lemma shows that \(\tilde{V}_k\) deviates from \(QV_k\) with the error \(O(\|\tilde{B}_k^{-1}\| \epsilon)\) and \(\tilde{V}_k = QV_k\) in exact arithmetic holds no longer. Using (3.8), we can rewrite (3.1) as

\[
(3.10) \quad (I_m, 0_{m \times p}) QV_k = U_{k+1} B_k + F_k
\]

where

\[
(3.11) \quad F_k = \tilde{F}_k - (I_m, 0_{m \times p}) (\tilde{V}_k - QV_k).
\]

Then from (3.4) and (3.8) we have \(\|F_k\| = O(\|\tilde{B}_k^{-1}\| \epsilon)\). Premultiplying (3.2) by \(Q^T\) and exploiting \((I_m, 0_{m \times p}) QV_k = Q_A V_k\) straightforwardly yields the following result,
which is the corresponding lower Lanczos bidiagonalization of \( Q_A \) in finite precision resulting from the JBD process.

**Theorem 3.1.** Suppose that the inner least squares problem (2.6) is solved accurately. In finite precision, we have

\[
\begin{align*}
Q_A V_k &= U_{k+1} B_k + F_k, \\
Q_A^T U_{k+1} &= V_k B_k^T + \alpha_k v_k + G_{k+1},
\end{align*}
\]

where \( G_{k+1} = Q^T \tilde{G}_{k+1} \) with \( \tilde{G}_{k+1} \) in (3.2) and \( \| F_k \| = O(\| B_k^{-1} \| \epsilon) \), \( \| G_{k+1} \| = O(\epsilon) \).

This theorem indicates that the error term \( F_k \) is amplified gradually once \( \| B_k^{-1} \| \) grows with \( k \). When \( Q_A \) is rectangular, i.e., \( m > n \), theoretically we cannot control the size of \( \| B_k^{-1} \| \), as shown now: from the second relation in (2.4), we obtain

\[
U_k^T Q_A Q_A^T U_k = B_k^T B_k,
\]

indicating that the eigenvalues of \( B_k^T B_k \), i.e., the squares of the singular values of \( B_k \), are the Ritz values of the singular matrix \( Q_A Q_A^T \) with respect to \( \text{span}(U_k) \) and lie between the largest and smallest eigenvalues of the singular matrix \( Q_A Q_A^T \). Notice that the Krylov subspace generated by \( u_1, Q_A Q_A^T u_1, \ldots, (Q_A Q_A^T)^{k-1} u_1 \). Then the smallest eigenvalue of \( B_k^T B_k \) converges to the zero eigenvalue of \( Q_A Q_A^T \) as \( k \) increases, so that \( \| B_k^{-1} \| \) may become uncontrollably large; on the other hand, for \( Q_A \) flat or square, i.e., \( m \leq n \), and having full row rank, however, such a phenomenon definitively cannot occur, and the smallest eigenvalue of \( B_k^T B_k \) is bounded from below by the smallest positive one of \( Q_A Q_A^T \). In this case, \( \| B_k^{-1} \| \) is always uniformly bounded but possibly large when \( Q_A \) is ill conditioned. We refer the reader to [11] on a detailed analysis on \( B_k \) and its singular values, which is closely related to and play a critical role in the conjugate gradient minimal error (CGME) method for solving least squares problems and linear discrete ill-posed problems. As a result, in finite precision, the the JBD process for computing \( U_{k+1}, V_k \) and \( B_k \) may be no longer equivalent to the lower Lanczos bidiagonalization of \( Q_A \), where the rounding error term in the place of \( F_k \) is \( O(\| Q_A \| \epsilon) = O(\epsilon) \) in size.

Similarly, from (1.5) and the first relation in (2.5) we have

\[
V_k^T Q_L Q_L V_k = \tilde{B}_k^T \tilde{B}_k.
\]

Since \( \text{span}(V_k) \) is the Krylov subspace generated by \( v_1, Q_L^T Q_L v_1, \ldots, (Q_L^T Q_L)^{k-1} v_1 \), we can make a similar analysis to the above. Specifically, if \( Q_L \) is rectangular or square and of full column rank, then the smallest singular value of \( B_k \) converges to the smallest one of \( Q_L \) from above as \( k \) increases, and it is bounded from below by it, meaning that \( \| B_k^{-1} \| \) is controllable; if \( Q_L \) is flat, then the smallest singular value of \( B_k \) converges to zero as \( k \) increases, causing that \( \| B_k^{-1} \| \) cannot be controlled and become large as \( k \) increases.

Note that the orders of \( Q_A \) and \( Q_L \) are the same as those of \( A \) and \( L \), respectively. The above analysis and assertions suggest us to first check the orders of \( A \) and \( L \) and then perform the JBD process on either \( \{ A, L \} \) or \( \{ L, A \} \) when attempting to ensure that the resulting \( \| B_k^{-1} \| \) and \( \| B_k^{-1} \| \) are bounded whenever possible. As will be seen later, their boundedness is desirable for the JBD process and the JBD method for the GSVD computation in finite precision.

In finite precision, we next prove that relation (2.12) holds within \( O(\epsilon) \), which is important to design an efficient and reliable algorithm for the GSVD computation.
To this end, we first establish upper bounds for $\|B_k\|$ and $\|\hat{B}_k\|$. From (3.1) and (3.3), at the $i$-th step we have

\[(3.14) \quad \hat{v}_i(1 : m) = \alpha_i u_i + \beta_{i+1} u_{i+1} + \hat{f}_i,\]

\[(3.15) \quad (-1)^{i-1} \hat{v}_i(m + 1 : m + p) = \hat{\alpha}_i \hat{u}_i + \hat{\beta}_{i-1} \hat{u}_{i-1} + \hat{f}_i.\]

Thus $\|\alpha_i u_i + \beta_{i+1} u_{i+1}\|^2 = \|\hat{v}_i(1 : m) - \hat{f}_i\|^2$, which leads to

\[(3.16) \quad \alpha_i^2 + \beta_{i+1}^2 = \|\hat{v}_i(1 : m)\|^2 + \|\hat{f}_i\|^2 - 2 \hat{f}_i^T \hat{v}_i(1 : m) - 2 \alpha_i \beta_{i+1} u_{i+1}^T u_i \leq 1 + O(c_1(m, n)\epsilon),\]

where we have used (3.5). Similarly, we obtain

\[(3.17) \quad \hat{\alpha}_i^2 + \hat{\beta}_{i-1}^2 \leq 1 + O(c_2(p, n)\epsilon).\]

Therefore, we have established the following lemma.

**Lemma 3.2.** In finite precision, we have\(^3\)

\[(3.18) \quad \|B_k\| \leq \sqrt{2} \max_{1 \leq i \leq k} (\alpha_i^2 + \beta_{i+1}^2)^{1/2} \leq \sqrt{2} + O(c_1(m, n)\epsilon),\]

\[(3.19) \quad \|\hat{B}_k\| \leq \sqrt{2} \max_{1 \leq i \leq k} (\hat{\alpha}_i^2 + \hat{\beta}_{i-1}^2)^{1/2} \leq \sqrt{2} + O(c_2(p, n)\epsilon).\]

We are ready to derive an important relationship between $B_k$ and $\hat{B}_k$ in finite precision, which was presented in [12, Theorem 3.1]. Because of its importance, here we give a simpler proof for the completeness.

**Theorem 3.2.** With the hypothesis of Theorem 3.1, in finite precision we have

\[(3.20) \quad B_k^T B_k + \hat{B}_k^T \hat{B}_k = I_k + E_k,\]

where $B_k = \hat{B}_k D_k$ with $D_k = \text{diag}(1, -1, \ldots, (-1)^{k-1})$, and $E_k$ is symmetric tridiagonal with its nonzero elements being $O(c_3(m, n, p)\epsilon)$ and $c_3(m, n, p) = c_1(m, n) + c_2(p, n)$ in size.

**Proof.** Since

\[
B_k^T B_k = \begin{pmatrix}
\alpha_1^2 + \beta_2^2 & \alpha_2 \beta_2 & & \\
\alpha_2 \beta_2 & \alpha_2^2 + \beta_3^2 & & \\
& \ddots & \ddots & \\
& & \alpha_k \beta_k & \alpha_k^2 + \beta_{k+1}^2
\end{pmatrix},
\]

\[
\hat{B}_k^T \hat{B}_k = \begin{pmatrix}
\hat{\alpha}_1^2 & \hat{\alpha}_1 \hat{\beta}_1 & & \\
\hat{\alpha}_1 \hat{\beta}_1 & \hat{\alpha}_2^2 + \hat{\beta}_1^2 & & \\
& \ddots & \ddots & \\
& & \hat{\alpha}_{k-1} \hat{\beta}_{k-1} & \hat{\alpha}_{k-1}^2 + \hat{\beta}_{k-1}^2
\end{pmatrix}
\]

are symmetric tridiagonal, $B_k^T B_k$ and $E_k$ in (3.20) are too.

\(^3\)Here we use the result of an exercise from [8, Chapter 6, Problem 6.14], which gives an upper bound for the $p$-norm of a row/column sparse matrix.
For the diagonal part, in finite precision, we have
\[ \tilde{\beta}_i = (\alpha_{i+1} \beta_{i+1} / \alpha_i)(1 + \rho_i), \]
where \(|\rho_i| = O(\epsilon)\) [8, Lemma 3.1], leading to
\[ \alpha_{i+1} \beta_{i+1} = \tilde{\alpha}_i \tilde{\beta}_i - \alpha_{i+1} \beta_{i+1} \rho_i. \]

From (3.16) we have
\[ \alpha_{i+1} \beta_{i+1} \leq \frac{\alpha_i^2 + \beta_i^2}{2} \leq \frac{2[1 + O(c_1(m, n)\epsilon)]}{2} = 1 + O(c_1(m, n)\epsilon). \]

Therefore, we obtain
\[ (3.21) \quad \alpha_{i+1} \beta_{i+1} = \tilde{\alpha}_i \tilde{\beta}_i + \gamma_i, \]
where \(|\gamma_i| \leq [1 + O(c_1(m, n)\epsilon)]\epsilon = O(\epsilon). \]

For the subdiagonal part, by taking norms in (3.14) and (3.15), we have
\[ \|\tilde{v}_i(1 : m)\|^2 + \|\tilde{v}_i(m + 1 : m + p)\|^2 \]
\[ = \|\alpha_i u_i + \beta_{i+1} u_{i+1} + \tilde{f}_i\|^2 + \|\tilde{\alpha}_i \tilde{u}_i + \tilde{\beta}_{i-1} \tilde{u}_{i-1} + \tilde{f}_{i-1}\|^2 \]
\[ = \alpha_i^2 + \beta_{i+1}^2 + 2\alpha_i \beta_{i+1} u_i^T u_{i+1} + 2\alpha_i u_i^T \tilde{f}_i + 2\beta_{i+1} u_{i+1}^T \tilde{f}_i + \|\tilde{f}_i\|^2 \]
\[ + \hat{\alpha}_i^2 + \hat{\beta}_{i-1}^2 + 2\hat{\alpha}_i \hat{\beta}_{i-1} \tilde{u}_i^T \tilde{u}_{i-1} + 2\hat{\alpha}_i \tilde{u}_i^T \tilde{f}_i + 2\hat{\beta}_{i-1} \tilde{u}_{i-1}^T \tilde{f}_i + \|\tilde{f}_{i-1}\|^2. \]

From (3.16) and (3.17) we obtain
\[ \alpha_i + \beta_{i+1} \leq \sqrt{2(\alpha_i^2 + \beta_{i+1}^2)} \leq \sqrt{2} + O(c_1(m, n)\epsilon), \]
\[ \hat{\alpha}_i + \hat{\beta}_{i-1} \leq \sqrt{2(\hat{\alpha}_i^2 + \hat{\beta}_{i-1}^2)} \leq \sqrt{2} + O(c_2(p, n)\epsilon), \]
showing that
\[ |2\alpha_i u_i^T \tilde{f}_i + 2\beta_{i+1} u_{i+1}^T \tilde{f}_i + \|\tilde{f}_i\|^2| \leq \sqrt{2} + O(c_2(p, n)\epsilon) \]
\[ = O(2(\alpha_i + \beta_{i+1})\epsilon) + O(2(\hat{\alpha}_i + \hat{\beta}_{i-1})\epsilon) = O(\epsilon), \]
where we have neglected the higher order term \(O(\epsilon^2)\). Exploiting (3.5) and (3.6), we obtain
\[ |2\alpha_i \beta_{i+1} u_i^T u_{i+1} + 2\hat{\alpha}_i \hat{\beta}_{i-1} \tilde{u}_i^T \tilde{u}_{i-1}| = O(c_3(m, n, p)\epsilon) \]
with \(c_3(m, n, p) = c_1(m, n) + c_2(p, n)\). Since
\[ 1 = \|\tilde{v}_i\|^2 = \|\tilde{v}_i(1 : m)\|^2 + \|\tilde{v}_i(m + 1 : m + p)\|^2, \]
we have
\[ (3.22) \quad \alpha_i^2 + \beta_{i+1}^2 + \hat{\alpha}_i^2 + \hat{\beta}_{i-1}^2 = 1 + O(c_3(m, n, p)\epsilon). \]

Combining (3.21) with (3.22) gives rise to (3.20).
of $B_k$ and $\tilde{B}_k$ can be determined each other with the error $O(\epsilon)$, it can be used to design algorithms for the GSVD computation. Therefore, if some extreme generalized singular values of $\{A, L\}$ are desired, then, except the approach that computes the generalized singular values of $\{B_k, \tilde{B}_k\}$ and uses extreme ones to approximate the corresponding ones of $\{A, L\}$, an alternative is to compute the singular values of $B_k$ or $\tilde{B}_k$ (or equivalently $B_k$) to obtain approximate generalized singular values. For a convergence analysis of the singular values of $B_k$ to some of $Q_A$ and more details, we refer the reader to [10, 11]. We will propose the JBD method for the GSVD computation and consider some details in Section 4, where we will revisit (3.20).

Since $B_k$ and $\tilde{B}_k$ have full column rank, by (3.20) we have

$$(B_k^T)^{\dagger}(B_k^T B_k + \tilde{B}_k^T B_k)B_k^{-1} = (B_k^T)^{\dagger}B_k^{-1} + (B_k^T)^{\dagger}E_k\tilde{B}_k^{-1}$$

which leads to

$$(\tilde{B}_k B_k^T)^{\dagger} = (B_k^T)^{\dagger}B_k B_k^{-1} + (B_k^T)^{\dagger}\tilde{B}_k^{-1} - (B_k^T)^{\dagger}E_k\tilde{B}_k^{-1}.$$  

Since $\tilde{B}_k^T = (B_k, \beta_k e_k)$, we have $||(B_k^T)^{\dagger}|| \leq ||\tilde{B}_k^{-1}||$. Notice that $||(B_k^T)^{\dagger}B_k^T|| = 1$. From (3.18) and (3.19), we obtain

$$||(\tilde{B}_k B_k^T)^{\dagger}|| \leq \sqrt{2}||\tilde{B}_k^{-1}|| + ||\tilde{B}_k^{-1}|| + c_0(\epsilon),$$

where

$$c_0(\epsilon) = ||\tilde{B}_k^{-1}|| ||\tilde{B}_k^{-1}|| O(c_3(m, n, p)\epsilon).$$

Since $\tilde{B}_k B_k^T = (\tilde{B}_k B_k, \beta_k + 1 \epsilon_k)$, by the interlacing property of singular values, we have $\sigma_k(\tilde{B}_k B_k) \leq \sigma_k(\tilde{B}_k B_k^T)$, where $\sigma_i(\cdot)$ denotes the $i$-th largest singular value of a matrix, proving that $||(\tilde{B}_k B_k^T)^{\dagger}|| \leq ||(\tilde{B}_k B_k)^{-1}||$. However, in our experiments, it has been found that $||(\tilde{B}_k B_k)^{-1}|| \leq c ||(\tilde{B}_k B_k)^{-1}||$ always holds with a modest constant $c = O(1)$, usually $c \leq 5$. Notice that $c_0(\epsilon)$ is much smaller than $||\tilde{B}_k^{-1}|| + ||\tilde{B}_k^{-1}||$. Therefore, in the sequel we will suppose and use the following upper bound for $||(\tilde{B}_k B_k)^{-1}||$:

$$||(\tilde{B}_k B_k)^{-1}|| \leq c \sqrt{2}||\tilde{B}_k^{-1}|| + ||\tilde{B}_k^{-1}||,$$

where $c > 1$ slightly.

We next establish a relationship between the JBD process for computing $\tilde{B}_k$ and the upper Lanczos bidiagonalization of $Q_L$ in finite precision.

**Theorem 3.3.** With the hypothesis of Theorem 3.1, in finite precision, we have

$$Q_L \hat{V}_k = \hat{U}_k \tilde{B}_k + \hat{F}_k,$$

$$Q_L^T \hat{U}_k = \hat{V}_k \tilde{B}_k^T + \hat{\beta}_k \hat{e}_k e_k + \hat{G}_k$$

with

$$||\hat{F}_k|| = O(||\tilde{B}_k^{-1}|| \epsilon),$$

$$||\hat{G}_k|| = O(c_4(m, n, p, k) \epsilon)$$

with

$$c_4(m, n, p, k) = ||\tilde{B}_k^{-1}|| + c_3(m, n, p)||\tilde{B}_k^{-1}||.$$
Proof. Recall the notation in (1.5), (2.10) and (2.5). Then exploiting Lemma 3.1, we can rewrite (3.3) as

\[(0_{p \times m}, I_p)\hat{V}_k = \hat{U}_k \hat{B}_k + \hat{F}_k,\]

where

\[(3.29) \quad \hat{F}_k = F_k - (0_{p \times m}, I_p)(\bar{V}_k - QV_k)D_k.\]

Therefore, (3.24) holds.

From (3.12) and (3.13), we obtain

\[(3.30) \quad Q_A^T Q_A V_k = Q_A^T U_{k+1} B_k + Q_A^T F_k \]

Premultiplying and postmultiplying \((3.30)\) yields

\[\sum \text{the above two equalities yields} \]

\[V_k = (Q_A^T Q_A + (Q_{2L}^T Q_{2L})) V_k \]

\[= V_k B_k^T B_k + Q_{2L}^T \hat{U}_k \hat{B}_k D_k + \alpha_{k+1} \beta_{k+1} \tilde{v}_{k+1} e_k^T + (G_{k+1} B_k + Q_A^T F_k + Q_{2L}^T \hat{F}_k D_k) \]

\[= V_k (I_k - D_k \hat{B}_k^T \hat{B}_k D_k + E_k) + Q_{2L}^T \hat{U}_k \hat{B}_k D_k + \alpha_{k+1} \beta_{k+1} \tilde{v}_{k+1} e_k^T \]

\[+ (G_{k+1} B_k + Q_A^T F_k + Q_{2L}^T \hat{F}_k D_k). \]

From this relation, \(\hat{V}_k = V_k D_k\) and \(D_k^2 = I_k\) it follows that

\[\hat{V}_k \hat{B}_k^T \hat{B}_k = Q_{2L}^T \hat{U}_k \hat{B}_k + \alpha_{k+1} \beta_{k+1} \tilde{v}_{k+1} e_k^T D_k + (G_{k+1} B_k + Q_A^T F_k + Q_{2L}^T \hat{F}_k D_k + V_k E_k) D_k \]

\[= Q_{2L}^T \hat{U}_k \hat{B}_k - (\alpha_{k+1} \beta \tilde{v}_{k+1} e_k^T + (G_{k+1} B_k + Q_A^T F_k + Q_{2L}^T \hat{F}_k D_k + V_k E_k) D_k, \]

which shows that

\[\hat{V}_k \hat{B}_k^T = Q_{2L}^T \hat{U}_k - \beta \tilde{v}_{k+1} e_k^T + E_1 + E_2, \]

where

\[E_1 = [(G_{k+1} B_k + V_k E_k) D_k - \gamma_k \tilde{v}_{k+1} e_k^T] \hat{B}_k^{-1}, \quad E_2 = (Q_A^T F_k D_k + Q_{2L}^T \hat{F}_k) \hat{B}_k^{-1}. \]

From (2.15), we have \(\|V_k\| \leq \sqrt{1 + \eta(V_k)}.\) Notice that \(\gamma_k\) in (3.21) satisfies \(|\gamma_k| = O(\epsilon)\) and the elements of \(\|E_k\|\) in (3.20) are \(O(c_3(m, n, p))\). Using the upper bounds for \(\|B_k\|\) in (3.18), we have

\[\|E_1\| = O(\varepsilon_1(m, n, p, k) \epsilon) \]

with \(\varepsilon_1(m, n, p, k) = (\sqrt{2} + c_3(m, n, p)) \|\hat{B}_k^{-1}\|\). Using the expressions of \(F_k, \hat{F}_k\) and \(\hat{V}_k - QV_k\) in (3.11), (3.29) and (3.9), respectively, we have

\[Q_A^T F_k D_k + Q_{2L}^T \hat{F}_k = (Q_A^T \quad Q_{2L}^T) \left( \begin{array}{c} F_k D_k \\ \hat{F}_k \end{array} \right) \]

\[= Q^T \left[ \left( \begin{array}{c} \hat{F}_k D_k \\ \hat{F}_k \end{array} \right) - \left( I_m \quad 0_{m \times p} \right) (V_k - QV_k) D_k \right] \]

\[= Q^T \left[ \left( \begin{array}{c} \hat{F}_k D_k \\ \hat{F}_k \end{array} \right) + (I_{m+p} - QQ^T) \hat{G}_k \hat{B}_k^{-1} D_k \right]. \]
From (3.23), we obtain
\[ \| \hat{B}_k^{-1} D_k \hat{B}_k^{-1} \| = \| (\hat{B}_k B_k)^{-1} \| \leq c \sqrt{2}(\| \hat{B}_k^{-1} \| + \| B_k^{-1} \|). \]

Since \( \| \hat{B}_k^{-1} \| = \| \hat{B}_k^{-1} \| \), it holds that
\[ \| E_2 \| = O(\bar{e}_2(k)\epsilon) \]

with \( \bar{e}_2(k) = c \sqrt{2}(\| \hat{B}_k^{-1} \| + \| B_k^{-1} \|) + \| \hat{B}_k^{-1} \|. \) Letting \( \hat{G}_k = -E_1 - E_2 \) leads to the desired result. \[ \Box \]

Notice that (3.24) and (3.25) are the corresponding versions of (2.5) in the presence of rounding errors. Therefore, this theorem indicates that the JBD process for computing \( \hat{U}_k \), \( \hat{V}_k \) and \( \hat{B}_k \) is no longer equivalent to the standard upper Lanczos bidiagonalization of \( Q_L \) with the rounding error \( O(\| Q_L \|\epsilon) = O(\epsilon) \) in finite precision, since the error terms \( \hat{F}_k \) and \( \hat{G}_k \) are amplified gradually once \( \| \hat{B}_k^{-1} \| \) and \( \| \hat{B}_k^{-1} \| \) grow as \( k \) increases.

In summary, unlike standard lower and upper Lanczos bidiagonalizations of \( Q_A \) and \( Q_L \) in finite precision, the JBD process in finite precision is lower and upper Lanczos bidiagonalizations with gradually growing error terms, where the growths of the error terms are dictated by \( \| \hat{B}_k^{-1} \| \) and \( \| \hat{B}_k^{-1} \| \) separately.

3.2. Loss of orthogonality of the Lanczos vectors. It is well known that, for Lanczos bidiagonalization, the numerical orthogonality of Lanczos vectors is gradually lost due to the influence of rounding errors. Once the orthogonality is lost at one iteration, the errors will propagate to later steps, which leads to the more loss of orthogonality of subsequently computed Lanczos vectors [18, 30]. For the JBD process, there is similar loss of orthogonality of each of the three sets of basis vectors. As it will turn out, the orthogonality levels of \( U_{k+1} \), \( \hat{V}_k \) and \( \hat{U}_k \) are closely related and interact. Below we prove how the orthogonality level of \( \hat{U}_k \) is affected by those of both \( U_{k+1} \) and \( \hat{V}_k \).

**Theorem 3.4.** With the hypothesis of Theorem 3.1, in finite precision, we have

\[ (3.31) \quad \eta(\hat{U}_k) \leq \| \hat{B}_k^{-1} \|^{2} \eta(\hat{V}_k) + 2\eta(U_{k+1}) + O(c_3(m, n, p)\epsilon). \]

**Proof.** From (3.1) and (3.3), we have
\[ \hat{V}_k = \begin{pmatrix} U_{k+1}B_k \\ \hat{U}_kB_k \end{pmatrix} + \begin{pmatrix} \hat{F}_k \\ \hat{F}_kD_k \end{pmatrix}, \]
which shows that
\[ (3.32) \quad \hat{V}_k^T \hat{V}_k = B_k^T U_{k+1}^T U_{k+1} B_k + B_k^T \hat{U}_k^T \hat{U}_k B_k + E_3, \]

where
\[ E_3 = B_k^T U_{k+1}^T \hat{F}_k + B_k^T \hat{U}_k^T \hat{F}_k P + \hat{F}_k^T U_{k+1} B_k + \hat{F}_k^T \hat{U}_k B_k + \hat{F}_k^T \hat{F}_k + P \hat{F}_k^T \hat{F}_k D_k. \]

From (3.20), we obtain
\[ I_k - \hat{V}_k^T \hat{V}_k = B_k^T (I_{k+1} - U_{k+1}^T U_{k+1}) B_k + B_k^T (I_k - \hat{U}_k^T \hat{U}_k) B_k - E_k - E_3, \]
which, together with (3.32), yields

\[(3.33) \quad I_k - \tilde{U}_k^T \tilde{U}_k = B_k^{-T} [(I_k - \tilde{V}_k^T \tilde{V}_k) - B_k^T (I_{k+1} - U_{k+1}^T U_{k+1})] B_k + E_k + E_3 \bar{B}_k^{-1}. \]

Notice that \(\| U_{k+1} \| \leq (1 + \eta(U_{k+1}))^{1/2} \) and \(\| \tilde{U}_k \| \leq (1 + \eta(\tilde{U}_k))^{1/2} \). Using the bounds for \(\| B_k \| \) and \(\| \bar{B}_k \| \) in (3.18) and (3.19), respectively, by a simple calculation, we obtain

\[\| E_3 \| = O(\epsilon).\]

Using the bound for \(\| B_k \| \), we have

\[\| B_k^T (I_{k+1} - U_{k+1}^T U_{k+1}) B_k \| \leq \| B_k \| \| I_{k+1} - U_{k+1}^T U_{k+1} \| \]
\[\leq 2 \| I_{k+1} - U_{k+1}^T U_{k+1} \| + O(c_1 (m, n) \epsilon).\]

Taking norms in (3.33) proves the desired result. \(\Box\)

The above theorem indicates that as long as \(\bar{B}_k \) is not ill conditioned, the orthogonality of \(\tilde{U}_k \) is as good as those of \(U_{k+1} \) and \(\tilde{V}_k \). Therefore, it is only necessary to perform some sort of reorthogonalization strategies to maintain desired orthogonality levels of \(U_{k+1} \) and \(\tilde{V}_k \).

The following result shows that the orthogonality levels of the long \(\tilde{V}_k \in \mathbb{R}^{(m+p) \times k} \) and the short \(V_k \in \mathbb{R}^{p \times k} \) are the same within \(O(\epsilon) \) under some mild condition.

**Theorem 3.5.** With definition (2.14), it holds that

\[(3.34) \quad | \eta(\tilde{V}_k) - \eta(V_k) | = O(\| \bar{B}_k^{-1} \| c^2).\]

**Proof.** From (3.9), we have

\[\tilde{V}_k^T (I_{m+p} - QQ^T) \tilde{V}_k = \tilde{V}_k^T (QV_k) = \tilde{V}_k^T (QQ^T - I_{m+p}) \tilde{V}_k \tilde{B}_k^{-1}\]
\[= -[I_{m+p} - QQ^T] \tilde{V}_k^T \tilde{B}_k^{-1}\]
\[= \tilde{B}_k^{-T} \tilde{G}_k (I_{m+p} - QQ^T) \tilde{G}_k \tilde{B}_k^{-T}.\]

Thus

\[I_k - \tilde{V}_k^T \tilde{V}_k = I_k - \tilde{V}_k^T QQ^T \tilde{V}_k = I_k - \tilde{V}_k^T \tilde{V}_k + \tilde{V}_k^T (I_{m+p} - QQ^T) \tilde{V}_k\]
\[= (I_k - \tilde{V}_k^T \tilde{V}_k) + \tilde{B}_k^{-T} \tilde{G}_k (I_{m+p} - QQ^T) \tilde{G}_k \tilde{B}_k^{-T}.\]

Therefore, (3.34) holds. \(\Box\)

This theorem shows that provided that \(\| \tilde{B}_k^{-1} \| \) is not too big, say no more than \(\epsilon^{-1/2} \), we have \(| \eta(\tilde{V}_k) - \eta(V_k) | = O(\epsilon) \). Therefore, it is only necessary to maintain the same orthogonality level of \(V_k \) in order to make \(\tilde{V}_k \) achieve a desired orthogonality level. From (3.31), this shows that we only need to maintain desired orthogonality levels of \(U_{k+1} \) and \(V_k \) so as to make \(\tilde{U}_k \) have a desired orthogonality level.

**4. The JBD method for the GSVD computation.** In this section, we review how to use the JBD process to compute some extreme GSVD components of \(\{A, L\} \) \[37\], which leads to the JBD method for the large GSVD computation, and make an analysis on the convergence of the approximate generalized singular values in finite precision by exploiting the previous results.
4.1. The JBD method. For ease of presentation, we do not take into account rounding errors when computing the GSVD of \( \{B_k, \tilde{B}_k\} \) or the SVD of \( B_k \) or \( \tilde{B}_k \), that is, we assume that the compact SVD of \( B_k \) is computed accurately:

\[
B_k = P_k \Theta_k W_k^T, \quad \Theta_k = \text{diag}(c_1^{(k)}, \ldots, c_k^{(k)}), \quad 1 \geq c_1^{(k)} > \cdots > c_k^{(k)} \geq 0,
\]

where \( P_k = (p_1^{(k)}, \ldots, p_k^{(k)}) \in \mathbb{R}^{(k+1) \times k} \) is orthonormal and \( W_k = (w_1^{(k)}, \ldots, w_k^{(k)}) \in \mathbb{R}^{k \times k} \) is orthogonal. The SVD \((4.1)\) can be obtained by a standard SVD algorithm since \( B_k \) is small sized. Then we have \( k \) approximate generalized singular values \( \{c_i^{(k)}, (1 - (c_i^{(k)})^2)^{1/2}\} \), \( i = 1, 2, \ldots, k \) of \( \{A, L\} \), and the approximate right generalized singular vectors are the \( x_i^{(k)} = \frac{R^{-1}V_k w_i^{(k)}}{\sqrt{c_i^{(k)}}} \) and the approximations to the left generalized singular vectors \( p_i^{A} \) are \( y_i^{(k)} = U_{k+1} p_i^{(k)} \). Among these \( k \) approximations, we pick up a few largest and/or smallest ones as approximations to the largest and/or smallest \( c_i/s_i \) and the corresponding \( x_i \) and \( p_i^{A} \).

If we also want to compute an approximation of the left generalized singular vector \( p_i^{L} \), we need to compute the SVD of \( B_k \). From \((2.12)\), it is known that \((B_k^T, \tilde{B}_k^T)^T\) is column orthonormal. Therefore, the CS decomposition of the pair \( \{B_k, \tilde{B}_k\} \) is its GSVD, and that the right singular vectors of \( B_k \) and \( \tilde{B}_k \) are identical. As a result, we can assume that the SVD of \( \tilde{B}_k \) is

\[
\tilde{B}_k = \tilde{P}_k \Psi_k W_k^T, \quad \Psi_k = \text{diag}(\tilde{s}_1^{(k)}, \ldots, \tilde{s}_k^{(k)}), \quad 0 \leq \tilde{s}_1^{(k)} < \cdots < \tilde{s}_k^{(k)} \leq 1,
\]

where \( \tilde{P}_k = (\tilde{p}_1^{(k)}, \ldots, \tilde{p}_k^{(k)}) \in \mathbb{R}^{k \times k} \) and \( W_k = (w_1^{(k)}, \ldots, w_k^{(k)}) \in \mathbb{R}^{k \times k} \) are orthogonal. Then \( z_i^{(k)} = \tilde{U}_k \tilde{p}_i^{(k)} \) is an approximation to \( p_i^{L} \). The approximate generalized singular values and the corresponding approximate right generalized singular vectors are \( \{1 - (z_i^{(k)})^2)^{1/2}, \tilde{s}_i^{(k)}\} \) and \( \frac{R^{-1}V_k w_i^{(k)}}{\sqrt{\tilde{s}_i^{(k)}}} \), respectively. We have seen that the approximate right generalized singular vectors obtained by the SVDs of \( B_k \) and \( \tilde{B}_k \) are the same, as expected. We also comment that if the JBD process is performed in exact arithmetic then mathematically \( \tilde{s}_i^{(k)} = s_i^{(k)} = \sqrt{1 - (c_i^{(k)})^2} \).

Alternatively, we compute the GSVD of the pair \( \{B_k, \tilde{B}_k\}: 

\[
B_k = P_k C_k W_k^T, \quad \tilde{B}_k = \tilde{P}_k S_k W_k^T,
\]

where \( C_k = \text{diag}(c_1^{(k)}, \ldots, c_k^{(k)}) \) and \( S_k = \text{diag}(s_1^{(k)}, \ldots, s_k^{(k)}) \), and \( P_k \) and \( \tilde{P}_k \) are as those defined in \((4.1)\) and \((4.2)\). The approximate generalized singular values are \( \{c_i^{(k)}, s_i^{(k)}\} \) or \( c_i^{(k)}/s_i^{(k)} \), the corresponding left approximate generalized singular vectors for \( A \) and \( L \) are \( U_{k+1} p_i^{(k)} \) and \( \tilde{U}_k \tilde{p}_i^{(k)} \), respectively, and the right approximate generalized singular vectors are \( x_i^{(k)} = Z_k w_i^{(k)} = R^{-1}V_k w_i^{(k)} \).

We remark that, in finite precision, the \( c_i^{(k)} \) and \( s_i^{(k)} \) in the GSVD of \( \{B_k, \tilde{B}_k\} \) are computed with no loss of accuracy and satisfy \( (c_i^{(k)})^2 + (s_i^{(k)})^2 = 1 \) unconditionally within working precision, irrespective of their sizes. In contrast, it is easily justified from \((3.20)\) that if either of \( B_k \) and \( \tilde{B}_k \) is ill conditioned then \( (1 - (c_i^{(k)})^2)^{1/2} \) or \( (1 - (s_i^{(k)})^2)^{1/2} \) as the singular values of \( \tilde{B}_k \) or \( B_k \) may be inaccurate when \( (c_i^{(k)})^2 = 1 - O(\epsilon) \) or \( (s_i^{(k)})^2 = 1 - O(\epsilon) \), which corresponds to an ill-conditioned \( \tilde{B}_k \) or \( B_k \) with small singular values no more than \( O(\epsilon^{1/2}) \), respectively. In other words, if \( B_k \) is ill conditioned and has a singular value no more than \( O(\epsilon^{1/2}) \), one would compute it with no accuracy from the corresponding singular value of \( B_k \), and vice versa. In this case, the corresponding approximate generalized singular values may be quite inaccurate.
and even has no accuracy; for the accuracy and reliability, we suggest to compute the singular values \( c_i^{(k)} \) and \( s_i^{(k)} \) of both \( B_k \) and \( \bar{B}_k \) separately and use \( \{ c_i^{(k)}, s_i^{(k)} \} \) as approximations to some extreme \( \{ c_i, s_i \} \).

For the computation of \( x_i^{(k)} \), it is shown in [37] that the explicit inversion \( R^{-1} \) can be avoided by noticing that

\[
\begin{pmatrix} A & \bar{L} \end{pmatrix} x_i^{(k)} = QRR^{-1}V_k w_i^{(k)} = \tilde{V}_k w_i^{(k)}.
\]

Then, solving the corresponding consistent linear system by an iterative solver, e.g., the LSQR algorithm, we obtain \( x_i^{(k)} \).

### 4.2. Convergence, accuracy and reorthogonalization.

In the presence of rounding errors, the behavior of the JBD algorithm may deviate from that in exact arithmetic. As mentioned previously, we only consider the rounding errors in the JBD process, and assume that the SVDs of \( B_k \) and \( \bar{B}_k \) are computed accurately, so are \( x_i^{(k)}, y_i^{(k)} \) and \( z_i^{(k)} \).

First, we investigate the convergence of the computed generalized singular values using the SVD of \( B_k \). Since \( c_i^2 + s_i^2 = 1 \), in order to compute the generalized singular value \( \{ c_i, s_i \} \), we only need to compute \( c_i \), which is a singular value of \( Q_A \). Note that \( c_i^{(k)} \), the singular value of \( B_k \), is a computed Ritz value of \( Q_A \), due to the property that the \( k \)-step JBD process for computing \( B_k \) is Lanczos bidiagonalization applied to \( Q_A \) with the rounding error \( O(\|B_k^{-1}\| \epsilon) \); see Theorem 3.1. In exact arithmetic, it is shown in [15] that the eigenvalues of \( B_k^T B_k \) are the Ritz values of \( Q_A^T Q_A \) with respect to the Krylov subspace generated by \( Q_A^T b, (Q_A^T Q_A)Q_A^T b, \ldots, (Q_A^T Q_A)^{k-1}Q_A^T b \) and the \( k \)-step lower bidiagonalization of \( Q_A \) is equivalent to the symmetric Lanczos process applied to \( Q_A^T Q_A \) and the starting vector \( Q_A^T b/\|Q_A^T b\| \) that generates the symmetric tridiagonal matrix \( B_k^T B_k \) and an orthonormal basis matrix \( V_k \) of the aforementioned Krylov subspace. Therefore, the convergence theory of the symmetric Lanczos method applies (cf. [27, 29]), and the singular values of \( B_k \) generally favor some largest and smallest ones of \( Q_A \). More convergence results and details have been given in [9, 10, 15]. In finite precision, typical convergence features of the symmetric Lanczos method carry over to our case, which include: (a) the computed Ritz values generally favor the extreme singular values of \( Q_A \), while interior singular values are hard to be approximated; (b) if the extreme singular values of \( Q_A \) are better separated one another, the corresponding computed Ritz values converge more rapidly. As a result, if we compute \( c_i \) by the SVD of \( B_k \), the computed Ritz values approximating the extreme generalized singular values of \( \{ A, L \} \) will first converge generally.

In finite precision, some of the singular values of \( B_k \) could be numerically multiple as the iteration number \( k \) increases, which may produce ghost approximations to some generalized singular values of \( \{ A, L \} \). A direct consequence is that a simple or genuine multiple generalized singular value of \( \{ A, L \} \) could be approximated by numerically multiple computed Ritz values, which could lead to a convergence delay of computed Ritz values. This phenomenon could occur only when the computed Lanczos vectors lose orthogonality and can be avoided by using some types of reorthogonalization strategies, such as full reorthogonalization or the more efficient one-sided reorthogonalization [32].

By Theorem 3.1, the JBD process for computing \( B_k \) is the lower Lanczos bidiagonalization of \( Q_A \) with the rounding error \( O(\|B_k^{-1}\| \epsilon) \) that is comparable to \( O(\epsilon) \) whenever \( \|B_k^{-1}\| \) is modest. If the JBD process is implemented with one-sided reorthogonalization of \( v_i \) such that the orthogonality level of \( V_k \) achieves \( O(\epsilon) \), exploiting
the backward error results on the Lanczos bidiagonalization with one-sided reorthogonalization [1, Theorem 5.2 and Corollary 5.1], we can deduce that the computed \( B_k \) is the exact one generated by the Lanczos bidiagonalization of a nearby matrix \( Q_A + E_k \) with \( \|E_k\| = O(\|B_k^{-1}\|\|e\|). \) Therefore, by the perturbation theory of the singular values [5, Corollary 8.6.2], the extreme singular values of \( Q_A \) can be computed with the ultimate accuracy \( O(\|B_k^{-1}\|\|e\|) \), and ghost Ritz values can be avoided.

It is known that a necessary orthogonality level of the computed basis vectors is the semiorthogonality for the symmetric Lanczos process [27, 30] and Lanczos bidiagonalization [18]. Based on Theorem 3.1 and [18, Theorem 5], it is straightforward to prove that the semiorthogonality suffices in finite precision.

**Theorem 4.1.** Assume that the compact QR factorizations of \( U_{k+1} \) and \( V_k \) are \( U_{k+1} = M_{k+1}R_{k+1} \) and \( V_k = N_kS_k \), where the diagonals of \( R_{k+1} \) and \( S_k \) are positive, and let \( \delta = O(\|B_k^{-1}\|\|e\|) \). If \( U_{k+1} \) and \( V_k \) satisfy the semiorthogonality

\[
(4.5) \quad \xi(U_{k+1}), \quad \xi(V_k) \leq \sqrt{\delta/(2k+1)}, \tag{4.5}
\]

then

\[
(4.6) \quad M_{k+1}^TQ_AN_k = B_k + \bar{E}_k,
\]

where the elements of \( \bar{E}_k \) are \( O(\delta) = O(\|B_k^{-1}\|\|e\|) \) in size.

Notice that \( M_{k+1}^TQ_AN_k \) is precisely the Ritz–Galerkin projection matrix of \( Q_A \) with respect to the left and right subspaces span(\( U_{k+1} \)) and span(\( V_k \)), whose singular values are the true Ritz values of \( Q_A \) with respect to these two subspaces in exact arithmetic, while the singular values of \( B_k \) are the computed Ritz values only when semiorthogonality is met. Theorem 4.1 indicates that once the orthogonality levels of \( U_{k+1} \) and \( V_k \) are below \( (\delta/(2k+1))^{1/2} \), the computed Ritz values are close to those true ones within \( O(\epsilon) \) provided that \( \|B_k^{-1}\| \) is modest. Since the true Ritz values are never ghosts provided that no breakdown occurs before iteration \( k \), we avoid the appearance of ghost computed Ritz values whenever \( U_{k+1} \) and \( V_k \) have semiorthogonality. Consequently, as long as true Ritz values are approximations to some singular values of \( Q_A \) with the accuracy \( O(\|B_k^{-1}\|\|e\|) \), the corresponding computed Ritz values have the same approximation accuracy too. In the meantime, it is easily justified that, when \( U_{k+1} \) and \( V_k \) have full orthogonality levels \( O(\epsilon) \), Theorem 4.1 holds with the norm of the error matrix in the right-hand side still being \( O(\|B_k^{-1}\|\|e\|) \). Therefore, the semiorthogonality of \( U_{k+1} \) and \( V_k \) suffices for computing generalized singular values accurately. We have made a detailed investigation on the JBD process with semiorthogonalization strategy and proposed an efficient partial reorthogonalization strategy in [12].

There is a corresponding counterpart of Theorem 4.1 for \( \tilde{B}_k \), as stated blow.

**Theorem 4.2.** Let \( \tilde{\delta} = O(c_4(m, n, p, k)\epsilon) \) with \( c_4(m, n, p, k) \) defined by (3.28), and the compact QR factorizations of \( \tilde{U}_k \) and \( V_k \) be \( \tilde{U}_k = \tilde{M}_k\tilde{R}_k \) and \( V_k = N_kS_k \), where

---

\(^2\)In Theorem 5 of Larsen [18], the right-hand side of (4.5) is \( \sqrt{\delta/k} \) instead of \( \sqrt{\delta/(2k+1)} \), but Larsen does not justify it rigorously. In fact, this result is a corresponding counterpart of [30, Theorem 4]. Since the \( k \)-step Lanczos bidiagonalization of \( Q_A \) with the starting vector \( b \) is equivalent to the \((2k+1)\)-step symmetric Lanczos process [2, §7.6.1] of \( \mathcal{C} = \begin{pmatrix} 0 & Q_A \\ Q_A^T & 0 \end{pmatrix} \) with the starting vector \( \tilde{b} = (b_0^T, 0) \), which holds not only in exact arithmetic but also in finite precision, the denominator in (4.5) should be \( 2k+1 \).
the diagonals of \( \hat{R}_k \) and \( S_k \) are positive. If \( \hat{U}_k \) and \( \hat{V}_k \) satisfy the semiorthogonality

\[
\xi(\hat{U}_k), \xi(\hat{V}_k) \leq \sqrt{\hat{\delta}/(2k+1)},
\]

then

\[
\bar{M}_k^T Q_L N_k = \bar{B}_k + \bar{E}_k,
\]

where the elements of \( \bar{E}_k \) are \( O(\hat{\delta}) = O(||\bar{B}_k^{-1}|| + ||\bar{B}_k^{-1}||\epsilon) \) in size.

Comparing Theorem 4.2 with Theorem 4.1, we find that Theorem 4.2 requires that \( ||\bar{B}_k^{-1}|| \) and \( ||\bar{B}_k^{-1}|| \) be controllable, stronger than the requirement of Theorem 4.1.

4.3. Residual norm and stopping criterion. Now we concentrate on designing an effective and efficient stopping criterion for the GSVD computation based on the JBD process. Still, we only assume rounding errors in the JBD process, and suppose that the other computations are exact. The following analysis focuses on computing some extreme GSVD components of \( \{A, L\} \) using the SVD of \( B_k \).

From the GSVD (2.2) of \( \{A, L\} \), it is known that the generalized eigenvalues \( \lambda \) of the symmetric generalized eigenvalue problem \( A^T Ax = \lambda L^T Lx \) are

\[
\infty, \ldots, \infty, (c_{q+1}/s_{q+1})^2, \ldots, (c_{q+l}/s_{q+l})^2, 0, \ldots, 0,
\]

and the corresponding generalized eigenvectors \( x \) are the right generalized singular vectors \( x \) of \( \{A, L\} \). The generalized eigenvalue problem \( A^T Ax = \lambda L^T Lx \) can be equivalently written as \( s_i^2 A^T Ax_i = c_i^2 L^T Lx_i \). Based on this equivalence, Zha in [37] uses the residual norm

(4.7) \[ ||r_i^{(k)}|| = ||((s_i^{(k)})^2 A^T A - (c_i^{(k)})^2 L^T L)x_i^{(k)}|| \]

to design a stopping criterion for an approximate generalized singular value pair \( \{c_i^{(k)}, s_i^{(k)}\} \) and the corresponding right vector \( x_i^{(k)} \), where \( (c_i^{(k)})^2 + (s_i^{(k)})^2 = 1 \). Clearly, the computation of \( ||r_i^{(k)}|| \) is expensive since it needs to compute \( x_i^{(k)} \) explicitly by solving a large scale least squares problem like (4.4) at each iteration \( k \) until the convergence occurs, where \( w_i^{(k)} \) depends on the approach used in the JBD method; see Section 4.1. In exact arithmetic, Zha [37] has proved a sharp bound:

(4.8) \[ ||r_i^{(k)}|| \leq ||R||\alpha_{k+1}\beta_{k+1}|e_k^T w_i^{(k)}| \]

with \( R \) defined in (1.1), so that \( ||R||\alpha_{k+1}\beta_{k+1}|e_k^T w_i^{(k)}| \) can be used to design a stopping criterion if \( ||R|| \) or its reasonable estimate is available. From (1.1), for \( C = (A^T, L^T)^T \)

we have \( ||R|| = ||C|| = \sigma_{\max}(C) \), the largest singular value of \( C \). Therefore \( ||r_i^{(k)}|| \) can be regarded as a relative residual norm of the approximate eigenvalue \( (c_i^{(k)})^2 / (s_i^{(k)})^2 \) and eigenvector \( x_i^{(k)} \) of the generalized eigenvalue problem \( s_i^2 A^T A = c_i^2 L^T Lx \). In finite precision, we can obtain the following upper bound for \( ||r_i^{(k)}|| \).

**Theorem 4.3.** Suppose that the inner least squares problem (2.6) is solved accurately and that \( x_i^{(k)} = R^{-1}V_k w_i^{(k)} \) with \( w_i^{(k)} \) being the right singular vector of \( B_k \) corresponding to its singular value \( c_i^{(k)} \). Then in finite precision it holds that

(4.9) \[ ||((s_i^{(k)})^2 A^T A - (c_i^{(k)})^2 L^T L)x_i^{(k)}|| \leq ||R||\left(\alpha_{k+1}\beta_{k+1}|e_k^T w_i^{(k)}| + O(||B_k^{-1}||\epsilon)\right). \]
Proof. From (3.30), we have
\[ Q_A^TQ_AV_k = VkB_k^2 + \alpha_{k+1}\beta_{k+1}v_{k+1}e_k^T + G_{k+1}B_k + Q_A^TF_k. \]
From (4.1), we have
\[ B_k^TW_k \Theta_k^2W_k^T. \]
Notice that \((s_i^{(k)})^2 = 1 - (c_i^{(k)})^2\) and \(x_i^{(k)} = R^{-1}V_ke_i\). Using the above two relations and (1.1), we obtain
\[
[(s_i^{(k)})^2A^T - (c_i^{(k)})^2(L^TL)x_i^{(k)} = [A^T - (c_i^{(k)})^2(A^T + L^TL)]R^{-1}V_ke_i
\]
\[ = R^T[Q_A^TQ_AV_k - (c_i^{(k)})^2V_kW_k]e_i
\]
\[ = R^T[\alpha_{k+1}\beta_{k+1} + e_k^{(k)} + (G_{k+1}B_k + Q_A^TF_k)w_i^{(k)}], \]
where \(e_i = \text{the } i\text{-th column of } I_k\). From Theorem 3.1, we have
\[ \|(G_{k+1}B_k + Q_A^TF_k)w_i^{(k)}\| = O(\|B_k^{-1}\|\|e\|). \]
Therefore, by taking norms in (4.10), we prove the desired result.

Using the same proof approach and based on Theorem 3.3, it is straightforward
to justify that this theorem still holds when we use the SVD of \(B_k\) to compute the
approximate generalized singular value \(\{(1 - (s_i^{(k)})^2)^{1/2}, s_i^{(k)}\}\) and approximate right
generalized singular vector \(x_i^{(k)} = R^{-1}V_ke_i\) with \(w_i^{(k)}\) being the right singular vector
of \(B_k\) corresponding to the singular value \(s_i^{(k)}\). Exploiting Lemma 3.1 and (3.1)–(3.3),
by a more involved analysis, we can prove that Theorem 3.3 holds too when we use the
GSVD of \(B_k, \alpha_k\) to compute the approximate generalized singular value \(c_i^{(k)}, s_i^{(k)}\)
and right generalized singular vector. We omit details here.

Let \((A^T, L^T)^T = C\), and recall the QR factorization (1.1) of \(C\). We have \(\|R\| = \|C\|\). If we perform Lanczos bidiagonalization on \(C\), several steps, then the largest
Ritz value is a reasonably good lower bound for \(\sigma_1(C)\). However, we should remind
that only a roughly good upper bound for \(\|C\|\) suffices for our use here. Notice
\[ \|R\|^2 = \|C\|^2 = \|CTC\| \leq \|A^TA\| + \|L^TL\| = \|A\|_1\|A\|_\infty + \|L\|_1\|L\|_\infty, \]
where \(\cdot_1\) and \(\cdot_\infty\) denote the 1-norm and the infinity norm, which is cheap to compute when \(A\) and \(L\) are explicitly stored in a certain sparse format. We then take the square
root of the right-hand side as an estimate for \(\|R\|\). Alternatively, it is simpler
to use \(\|C\|_1 \leq \|A\|_1 + \|L\|_1\) or \(\|C\|_\infty = \max\{\|A\|_\infty, \|L\|_\infty\}\) as a replacement of \(\|R\|\).
Since \(c_i^{(k)}w_i^{(k)}\) is available from the SVD of \(B_k\), the quantity \(\|R\|_1\|A\|_b\|L\|_b\|e_k^{(k)}\|\) can be used as a reliable stopping criterion, provided that the stopping tolerance for the
(relative) residual norm is not required to achieve the level of \(\epsilon\). Computationally, we
benefit very much from this criterion since we avoid the explicit computation of \(x_i^{(k)}\)
before the convergence. We will numerically confirm the reliability of the criterion.

5. Numerical experiments. We report numerical experiments to justify the results obtained. All the numerical experiments were performed on an Intel (R)
Core (TM) i7-7700 CPU 3.60GHz with the main memory 8GB using the Matlab
R2017a with the machine precision \(\epsilon = 2.22 \times 10^{-16}\) under the Microsowf Windows
10 64-bit system. For each matrix pair \(\{A, L\}\), we use \(b = (1, \ldots, 1)^T \in \mathbb{R}^m\) as the
starting vector of the JBD process, and each inner least squares problem (2.6) is solved
accurately by computing the QR factorization (1.1) and \(QQ^Tw\) for a given \(w\).
5.1. Examples for the JBD process in finite precision. We choose four matrix pairs to confirm the numerical behavior of the JBD process in finite precision. We construct the first pair \( \{ A, L_s \} \) as follows: Take \( n = 800 \) and \( C_A = \text{diag}(c) \), \( S_L = \text{diag}(s) \), where \( c = \left( \frac{3n}{2}, \frac{3n}{2} - 1, \ldots, \frac{n}{2} + 1 \right) / 2n \) and \( s = (\sqrt{1 - c_1^2}, \ldots, \sqrt{1 - c_2^2}) \). Let \( D \) be the symmetric orthogonal matrix generated by the MATLAB built-in function \( \text{d} = \text{gallery}('\text{orthog}',n,2) \). We then define \( A = C_A D \) and \( L = S_L D \). By construction, the \( i \)-th generalized singular value of \( \{ A, L \} \) is \( \{ c_i, s_i \} \) and the corresponding right vector \( x_i \) is the \( i \)-th column of \( D \), and the left generalized singular vectors \( p_i^L \) and \( p_i^S \) are the \( i \)-th column \( e_i \) of \( I_n, i = 1, \ldots, n \). The remaining three pairs use sparse matrices from [3], where

\[
L = L_1 = \begin{pmatrix}
1 & -1 & & \\
1 & -1 & & \\
& & \ddots & \\
& & & 1 & -1
\end{pmatrix} \in \mathbb{R}^{(n-1)\times n}
\]

with \( n = 712 \), which is the scaled discrete approximation of the first order derivative operator, and \( L = L_n = \text{diag}(l) \) with \( l = (2n, 2n - 1, \ldots, n + 1) / 1000 \), \( n = 3969 \).

Some properties of the four test matrix pairs are described in Table 1, where \( \kappa(A) = \|A\|\|A^T\| \) is the condition number of \( A \).

| \( A \) | \( m \times n \) | \( \kappa(A) \) | \( L \) | \( p \times n \) | \( \kappa(L) \) |
|------|------------|----------|------|------------|----------|
| \( A_c \) | 800 × 800 | 2.99 | \( L_s \) | 800 × 800 | 1.46 |
| well1850 | 1850 × 712 | 111.31 | \( L_1 \) | 711 × 712 | 453.27 |
| rd2048 | 2048 × 2048 | 2026.80 | \( \text{dw}2048 \) | 2048 × 2048 | 5301.50 |
| c-23 | 3969 × 3969 | 22795.9 | \( L_n \) | 3969 × 3969 | 1.9995 |

Figure 1 depicts the growths of \( \|F_k\| \) and \( \|G_{k+1}\| \) in (3.12) and (3.13) as the iteration number \( k \) increases from 1 to 150. By Theorem 3.1, we take \( O(\|B_k^{-1}\|\|\epsilon\|) = 10\|B_k^{-1}\|\|\epsilon\| \) for the four test problems, it is seen from Figure 1(a)–Figure 1(d) that \( \|F_k\| \) grows very slowly as \( k \) increases. For the four matrix pairs, \( O(\|B_k^{-1}\|\|\epsilon\|) \) is indeed a very good upper bound for \( \|F_k\| \) in ten times, and the growth trends of \( \|F_k\| \) and \( \|B_k^{-1}\| \) are similar. This indicates that the growth of \( \|F_k\| \) is mainly affected by the growth of \( \|B_k^{-1}\| \). Since \( QQ^T \tilde{u}_i \) is explicitly computed at each step in our experiments, \( \|G_{k+1}\| = O(\|\epsilon\|) \) remains almost unchanged.

Figure 2 depicts the growth of \( \|E_k\| = \|I_k - B_k^T \tilde{B}_k - \tilde{B}_k^T \tilde{B}_k\| \). Since the nonzero elements of \( E_k \) are \( O(c_3(m, n, p)\|\epsilon\|) \) in size, we use 100\( \|\epsilon\| \) as an upper bound for \( \|E_k\| \). For the four matrix pairs, we find that as \( k \) increases from 1 to 150, \( \|E_k\| \) is always at the level of \( \|\epsilon\| \) and the bound estimates it quite well, justifying (3.20).

Figure 3 depicts the growths of \( \|\tilde{F}_k\| \) and \( \|\tilde{G}_k\| \) in (3.24) and (3.25). By Theorem 3.3, we take \( O(\|B_k^{-1}\|\|\epsilon\|) = 10\|B_k^{-1}\|\|\epsilon\| \) and \( O((\|B_k^{-1}\| + \|\tilde{B}_k^{-1}\|)\|\epsilon\|) = 10(\|B_k^{-1}\| + \|\tilde{B}_k^{-1}\|)\|\epsilon\| \), respectively. From the figures, we see that \( O(\|B_k^{-1}\|\|\epsilon\|) \) and \( O((\|B_k^{-1}\| + \|\tilde{B}_k^{-1}\|)\|\epsilon\|) \) are indeed reasonable upper bounds for \( \|\tilde{F}_k\| \) and \( \|\tilde{G}_k\| \). The growths of \( \|\tilde{F}_k\| \) and \( \|\tilde{G}_k\| \) are critically affected by those of \( \|B_k^{-1}\| \) and \( \|B_k^{-1}\| + \|\tilde{B}_k^{-1}\| \), respectively. For the four matrix pairs, \( \|B_k^{-1}\| \) always grows slowly, but \( \|\tilde{B}_k^{-1}\| = \|\tilde{B}_k^{-1}\| \) grows faster for \( \{ \text{well1850}, L_1 \} \) than for the other three pairs. This is because \( L_1 \) is truly flat and
Fig. 1. Estimated error bound for $\|F_k\|$: (a) $\{A_c, L_s\}$; (b) $\{\text{well1850, } L_1\}$; (c) $\{\text{rdb2048, } \text{dw2048}\}$; (d) $\{c-23, L_n\}$.

Fig. 2. Error bound for $\|I_k - B_k^T B_k - B_k \bar{B}_k\|$: (a) $\{A_c, L_s\}$; (b) $\{\text{well1850, } L_1\}$; (c) $\{\text{rdb2048, } \text{dw2048}\}$; (d) $\{c-23, L_n\}$.
the smallest singular value of $\bar{B}_k$ converges to zero as $k$ increases, causing that $\|\bar{B}_k^{-1}\|$ is ultimately very large, as we have shown in almost one page after Theorem 3.1; in contrast, the smallest singular value of $\bar{B}_k$ converges to the nonzero smallest one of $L$ for the other three matrix pairs, and $\|\bar{B}_k^{-1}\|$ is uniformly bounded by the reciprocal of the smallest singular value of $L$.

Figure 4 depicts the orthogonality level of $\hat{U}_k$ measured by $\eta(\hat{U}_k)$ as $k$ increases from 1 to 150. The upper bound for $\eta(\hat{U}_k)$ is (3.31), and we use $10\kappa$ as an estimate for $O(c_3(m,n,p)\kappa)$. We observe that the orthogonality of $\hat{U}_k$ will lose gradually. Particularly, for the test problem $\{\text{rdb2048, dw2048}\}$, the columns of $\hat{U}_k$ lose orthogonality completely and become numerically linearly dependent after $k = 100$. The growth trends of $\eta(\hat{U}_k)$ and its bound resemble, meaning that the orthogonality level of $\hat{U}_k$ is affected not only by $\eta(U_k)$ and $\eta(\tilde{V}_k)$ but also by $\|\hat{B}_k^{-1}\|$.

5.2. Examples for the GSVD computation. We illustrate the numerical performance of the JBD method for computing a few extreme GSVD components of $\{A, L\}$. We will show the convergence behavior of the computed Ritz values and vectors, and justify the upper bound in (4.9).

Example 1. We show the convergence of the singular values, the computed Ritz values, of $B_k$ or $\bar{B}_k$. Take $m = n = p = 500$, and use 20 as an estimate for $O(c_3(m,n,p)\kappa)$. We observe that the orthogonality of $\hat{U}_k$ will lose gradually. Particularly, for the test problem $\{\text{rdb2048, dw2048}\}$, the columns of $\hat{U}_k$ lose orthogonality completely and become numerically linearly dependent after $k = 100$. The growth trends of $\eta(\hat{U}_k)$ and its bound resemble, meaning that the orthogonality level of $\hat{U}_k$ is affected not only by $\eta(U_k)$ and $\eta(\tilde{V}_k)$ but also by $\|\hat{B}_k^{-1}\|$.
the \(i\)-th large generalized singular value pair of \(\{A, L\}\) is \(\{c_i, s_i\}\).

Figure 5 depicts the convergence processes of the first six largest and smallest
Ritz values computed by the SVD of \(B_k\), respectively, where we implemented the JBD
process without and with reorthogonalization. The right vertical line indicates the
values of \(c_i\) for \(i = 1, \ldots, 500\), and the left and right panels exhibit the convergence
behaviors of the JBD method without and with reorthogonalization. We observe
from Figure 5(a) and Figure 5(c) that some of the converged Ritz values suddenly
jump to become a ghost and then converge to the next large or small singular values
after several iterations. Such a phenomenon repeats several times and corresponds
to spurious copies each time. More precisely, as Figure 5(a) indicates, the six largest
Ritz values gradually become numerically multiple and ultimately converge to the
single largest generalized singular value of \(\{A, L\}\) as \(k\) increases, of which five ones
are ghosts. Similarly, as Figure 5(c) shows, the six smallest Ritz values ultimately
converge to the two smallest generalized singular values of \(\{A, L\}\), of which the most
slowly converged Ritz value first converges to the seventh smallest generalized singular
value of \(\{A, L\}\), then suddenly jumps and starts to approximate the smallest one after
69 iterations, and the other five Ritz values finally become numerically multiple and
converge to the second smallest generalized singular value of \(\{A, L\}\) after nearly 170
iterations, meaning that four of these five ones are ghosts since then.

However, when the JBD process is performed with full reorthogonalization, the
convergence of the Ritz values changes and becomes regular, as Figure 5(b) and
Figure 5(d) indicate. In the right panels, the convergence behavior is much simpler
and is in accordance with theoretical analysis in exact arithmetic. It is clear that a
simple generalized singular value is approximated by Ritz values without ghosts. We
also observe from both the panels that the extreme Ritz values converge more quickly than relatively interior Ritz values, that is, the Ritz values closer to the right-most or left-most generalized singular values stabilize more early, which confirms the theory that the JBD method generally favors the extreme generalized singular values.

Figure 6 depicts the convergence processes of the first six smallest Ritz values computed by the SVD of $\bar{B}_k$, which corresponds to the first largest generalized singular values of $\{A, L\}$. The convergence behavior of the largest Ritz values by the SVD of $\bar{B}_k$ is similar and thus omitted. The right vertical line indicates the values of $s_i$. 
for \( i = 1, \ldots, 500 \). From Figure 6(a), we observe the “ghost” phenomenon that some converged Ritz values suddenly jump and then converge to the next small singular values after several iterations. More detailed convergence phenomena are similar to Figure 5(a) and Figure 5(c). Figure 6(b) shows the convergence of Ritz values with full reorthogonalization, from which it is clear that the JBD method converges regularly and there are no spurious copies. Figure 6(a)–Figure 6(b) demonstrate that the JBD method favors the extreme generalized singular values.

Example 2. We investigate the convergence of the approximate generalized singular values and vectors of \( \{A, L\} \), which are computed by using both the SVDs of \( B_k \) and \( \hat{B}_k \) and the GSVD of \( \{B_k, \hat{B}_k\} \). We test two matrix pairs. The first pair is the problem in Example 1, and the second pair \( \{dw256A, dw256B\} \) is an electromagnetic problem with \( m = n = p = 512 \) from the non-Hermitian Eigenvalue Problem Collection in the Matrix Market\(^3\), where \( \kappa(A) = 11490.4 \) and \( \kappa(L) = 3.7328 \).

We use the JBD method with full reorthogonalization to compute the largest generalized singular value and vectors. Instead of the SVD of the individual \( B_k \) or \( \hat{B}_k \), we compute the SVDs of \( B_k \) and \( \hat{B}_k \) simultaneously, and take \( \{c_1^{(k)}, \hat{s}_1^{(k)}\} \) to approximate \( \{c_1, s_1\} \), where \( c_1^{(k)} \) is the largest singular value of \( B_k \) and \( \hat{s}_1^{(k)} \) is the smallest singular value of \( \hat{B}_k \). The approximations to the right and left generalized singular vectors \( x_1 \) and \( p_1^A \) are computed from the SVD of \( B_k \), and the approximation to the left generalized singular vectors \( p_1^L \) is computed from the SVD of \( \hat{B}_k \). Alternatively, we also compute the largest GSVD components of these two matrix pairs using the GSVD of \( \{B_k, \hat{B}_k\} \) and obtain the approximation \( \{c_1^{(k)}, s_1^{(k)}\} \) to \( \{c_1, s_1\} \) and the approximations \( x_1^{(k)}, y_1^{(k)}, \hat{z}_1^{(k)} \) to \( x_1, p_1^A, p_1^L \).

We use the angle error

\[
\sin \theta_k = |s_1^{(k)} c_1 - s_1 c_1^{(k)}| \text{ or } |s_1^{(k)} c_1 - s_1 c_1^{(k)}|
\]

to measure the error between \( \{c_1^{(k)}, \hat{s}_1^{(k)}\} \) or \( \{c_1^{(k)}, s_1^{(k)}\} \) and \( \{c_1, s_1\} \) [34], where \( \theta_k \) denotes the angle between the vectors \( (c_1, s_1)^T \) and \( (c_1^{(k)}, \hat{s}_1^{(k)})^T \) or \( (c_1^{(k)}, s_1^{(k)})^T \). For the corresponding generalized singular vectors, we measure the errors

\[
\sin \angle(x_1, x_1^{(k)}), \quad \sin \angle(p_1^A, y_1^{(k)}), \quad \sin \angle(p_1^L, \hat{z}_1^{(k)}).
\]

Figure 8 draws the approximation processes of the approximate generalized singular values and vectors obtained by the SVDs of \( B_k \) and \( \hat{B}_k \) as \( k \) increases, while Figure 7 depicts the growths of \( \|B_k^{-1}\| \) and \( \|\hat{B}_k^{-1}\| \). We have found that, for these two matrix pairs, \( \|B_k^{-1}\| \) and \( \|\hat{B}_k^{-1}\| \) grow quite slowly and are very modest for Example 1 when \( k = 1 \sim 150 \) and for Example 2 when \( k = 1 \sim 150 \), respectively. The approximate GSVD components converge regularly, the JBD method converges fast, and all the errors achieve the level of \( \epsilon \) after twenty iterations for Example 1.

Figure 9 depicts the convergence processes of approximate GSVD components computed by the GSVD of \( \{B_k, \hat{B}_k\} \). In this figure, we also draw the curves of residual norms. Clearly, the computed results are very similar to those obtained by the SVDs of \( B_k \) and \( \hat{B}_k \) until the errors reach the level of \( \epsilon \).

Example 3. We show the residual norm and its upper bound (4.9). The matrix pair \( \{A, L\} \) is chosen to be \( \{A_{800}, L_{800}\} \) in Table 1, and we use the largest singular value of \( B_k \) to compute an approximation to the largest generalized singular value.

\(^3\)https://math.nist.gov/MatrixMarket
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Fig. 7. Growth of $\|B_k^{-1}\|$ and $\|\hat{B}_k^{-1}\|$: (a),(b) $\{A_{500}, L_{500}\}$ in Example 1; (c),(d) $\{dw256A, 256B\}$ in Example 2.

Fig. 8. Convergence processes of the approximate GSVD components: (a) $\{A_{500}, L_{500}\}$ in Example 1; (b) $\{dw256A, 256B\}$ in Example 2.

From the construction, we have $\|(A_{800}^T, L_{800}^T)^T\| = 1$, and the largest generalized singular value is $\{c_1, s_1\}$, where $c_1 = 0.75$ and $s_1 = \sqrt{1 - c_1^2}$.

We also display the convergence processes of the approximate generalized singular values by using both the angle error and relative error

$|c_1^{(k)}/s_1^{(k)} - c_1/s_1|/(c_1/s_1)$.

We draw the convergence histories of the approximate largest generalized singular value and the residual norm in Figure 10. From Figure 10(b), It is found that the approximate largest generalized singular value $c_1^{(k)}/s_1^{(k)}$ converges to $c_1/s_1$, and the
relative error curve shows that the approximation accuracy of \(c_i^{(k)}/s_i^{(k)}\) to \(c_i/s_i\) reaches \(O(\epsilon)\). We observe from Figure 10(a) that the residual norm and its upper bound are almost the same as \(k\) increases. The true residual norm decays until the level of \(\epsilon\), but the estimated upper bound stagnates at the level that is a little bit higher than \(\epsilon\), since the upper bound for \(\|r_i^{(k)}\|\) has a term \(O(\|B_k^{-1}\|\epsilon)\), which is considerably bigger than \(\epsilon\) when \(\|B_k^{-1}\| \approx 1\) considerably. For the case that \(\|B_k^{-1}\|\) remains modest, the term \(O(\|B_k^{-1}\|\epsilon)\) plays no role in the upper bound until the bound reaches \(O(\epsilon)\). Therefore, the upper bound \(\|R\|\alpha_{k+1}\beta_{k+1}|\epsilon_i^{(k)} w_i^{(k)}|\) can be used as a reliable stopping criterion for the JBD algorithm. We have seen that the angle errors and relative errors resemble very much, as is expected since \(c_i/s_i = O(1)\). We point out that, in large matrix computations, a (relative) stopping tolerance is usually \(O(\epsilon^{1/2})\). Therefore, provided that \(\|B_k^{-1}\| \leq O(\epsilon^{-1/2})\), our upper bound is a very reliable estimate for \(\|r_i^{(k)}\|\).

6. Conclusions and future work. We have made a numerical analysis of the JBD process on \(\{A, L\}\) in finite precision, and established relationships between it and respective lower and upper Lanczos bidiagonalizations of \(Q_A\) and \(Q_L\) in the presence of round-offs. The results have shown that the \(k\)-step JBD process for computing \(U_{k+1}, V_k\) and \(B_k\) is equivalent to the lower Lanczos bidiagonalization of \(Q_A\) with the error \(\delta = O(\|B_k^{-1}\|\epsilon)\), and it for computing \(\tilde{U}_{k+1}, V_k\) and \(\tilde{B}_k\) is equivalent to the upper Lanczos bidiagonalization of \(Q_L\) with the error \(\delta = O((\|B_k^{-1}\| + \|\tilde{B}_k^{-1}\|)\epsilon)\). We have
investigated the loss of orthogonality of the computed basis vectors and established an upper bound for the orthogonality level of $\eta(\bar{U}_k)$, showing that its orthogonality level is controlled by those of $\bar{U}_{k+1}$, $\bar{V}_k$, i.e., $V_k$, and the quantity $\|\bar{B}_k^{-1}\|$.

We have shown how to use the JBD process to compute a few extreme generalized singular values and vectors of $\{A, L\}$ and proposed a JBD method that obtains approximate generalized singular values and vectors using a few computational approaches, which include three approaches to obtain approximate generalized singular values and approximate right generalized singular vectors by computing the SVDs of $B_k$ and $\bar{B}_k$ and the GSVD of $\{B_k, \bar{B}_k\}$ and two approaches to obtain approximate left generalized singular vectors of $A$ and $L$ by computing either the left singular vectors of $B_k$ and $\bar{B}_k$ simultaneously or the left generalized singular vectors of $\{B_k, \bar{B}_k\}$. We have considered the convergence and accuracy of the approximate generalized singular values. The results have indicated that the generalized singular values of $B_k$ and $\bar{B}_k$ are as accurate as the true Ritz values of $Q_A$ and $Q_L$ with respect to the given subspaces within $O(\epsilon)$, provided that the basis vectors have semiorthogonality levels and $B_k$ and $\bar{B}_k$ are not ill conditioned. Under these conditions, it is only necessary to maintain the desired semiorthogonality in order to obtain the approximate GSVD components with the same accuracy as those obtained by the JBD method with full reorthogonalization. An efficient partial reorthogonalization strategy has been proposed in [12] for this purpose.

In the meantime, we have established a compact upper bound for the residual norm $\|r_i^{(k)}\|$ of an approximate generalized singular value and approximate right generalized singular vector in finite precision and shown that it can be used as a cheap and reliable stopping criterion without explicitly computing the approximate right generalized singular vector until the convergence occurs. Finally, we have reported numerical experiments to justify all the results obtained and assertions.

There remain some important issues. For instance, due to the limitation of storage, it is generally necessary to restart the JBD method. A commonly used restarting technique is the implicit restarting proposed in [33] for the eigenvalue problem and adapted to the SVD computation in [13, 14, 19]. How to adapt the implicit restart to the JBD method and develop efficient algorithms is very significant. Also, notice that the residual norm (4.7) is used to measure the convergence of the JBD method, which is the residual norm of an approximate generalized eigenpair $((c_i^{(k)}/s_i^{(k)})^2, x_i^{(k)})$ of $s_i^2 A^T A x_i = c_i^2 L^T L x_i$ and does not take approximate left generalized singular vectors $y_i^{(k)}$ for $A$ and $z_i^{(k)}$ for $L$ into account. A much more proper criterion is to measure the residual norm of the approximate GSVD components $\{c_i^{(k)}, s_i^{(k)}, x_i^{(k)}, y_i^{(k)}, z_i^{(k)}\}$, which, by the definition (2.3) of GSVD of $\{A, L\}$, is

$$\|r_i^{(k)}\| = \sqrt{\|A x_i^{(k)} - c_i^{(k)} y_i^{(k)}\|^2 + \|L x_i^{(k)} - s_i^{(k)} z_i^{(k)}\|^2 + \|s_i^{(k)} A^T y_i^{(k)} - c_i^{(k)} L^T z_i^{(k)}\|^2}.$$  

We need to establish reliable upper bounds for it in exact arithmetic and in finite precision so as to design an efficient stopping criterion for the GSVD computation.

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