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The joint bidiagonalization process with partial reorthogonalization

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Abstract
The joint bidiagonalization (JBD) process is a useful algorithm for the computation of the generalized singular value decomposition (GSVD) of a matrix pair. However, it always suffers from rounding errors, which causes the Lanczos vectors to lose their mutual orthogonality. In order to maintain some level of orthogonality, we present a semiorthogonalization strategy. Our rounding error analysis shows that the JBD process with the semiorthogonalization strategy can ensure that the convergence of the computed quantities is not affected by rounding errors and the final accuracy is high enough. Based on the semiorthogonalization strategy, we develop the joint bidiagonalization process with partial reorthogonalization (JBDPRO). In the JBDPRO algorithm, reorthogonalizations occur only when necessary, which saves a big amount of reorthogonalization work, compared with the full reorthogonalization strategy. Numerical experiments illustrate our theory and algorithm.

Keywords Joint bidiagonalization · GSVD · Lanczos bidiagonalization · Orthogonality level · Semiorthogonalization · Partial reorthogonalization · JBDPRO

Mathematics Subject Classification (2010) 15A18 · 65F15 · 65F25 · 65F50 · 65G50

1 Introduction

The joint bidiagonalization (JBD) process is a useful algorithm for computing some extreme generalized singular values and vectors for a large sparse or structured matrix pair $\{A, L\}$ [20, 28] where $A \in \mathbb{R}^{m\times n}$ and $L \in \mathbb{R}^{p\times n}$, as well as solving

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large-scale discrete ill-posed problems with general-form Tikhonov regularization [6–8]. First proposed by Zha [30], it iteratively reduces the matrix pair $\{A, L\}$ to an upper or lower bidiagonal form. It was later adapted by Kilmer [12] to jointly diagonalize $\{A, L\}$ to lower and upper bidiagonal forms.

Consider the compact QR factorization of the stacked matrix:

$$\begin{pmatrix} A \\ L \end{pmatrix} = QR = \begin{pmatrix} Q_A \\ Q_L \end{pmatrix} R, \tag{1.1}$$

where $Q \in \mathbb{R}^{(m+p)\times n}$ is column orthonormal and $R \in \mathbb{R}^{n\times n}$. We partition Q such that $Q_A \in \mathbb{R}^{m\times n}$ and $Q_L \in \mathbb{R}^{p\times n}$, so that $A = Q_A R$ and $L = Q_L R$. Applying the BIDIAG-1 procedure and BIDIAG-2 procedure [21], which correspond to the lower and upper Lanczos bidiagonalization processes [4], to Q_A and Q_L, respectively, we can reduce Q_A and Q_L to the following lower and upper bidiagonal matrices, respectively:

$$B_k = \begin{pmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \beta_3 & \ddots & \\ & & \ddots & \alpha_k \\ & & & \beta_{k+1} \end{pmatrix} \in \mathbb{R}^{(k+1)\times k}, \quad \widehat{B}_k = \begin{pmatrix} \hat{\alpha}_1 & \hat{\beta}_1 & & \\ & \hat{\alpha}_2 & \ddots & \\ & & \ddots & \hat{\beta}_{k-1} \\ & & & \hat{\alpha}_k \end{pmatrix} \in \mathbb{R}^{k\times k}. \tag{1.2}$$

The two processes produce four column orthonormal matrices, that is

$$U_{k+1} = (u_1, \ldots, u_{k+1}) \in \mathbb{R}^{m\times(k+1)}, \quad V_k = (v_1, \ldots, v_k) \in \mathbb{R}^{n\times k} \tag{1.3}$$

computed by the BIDIAG-1 algorithm, and

$$\widehat{U}_k = (\hat{u}_1, \ldots, \hat{u}_k) \in \mathbb{R}^{p\times k}, \quad \widehat{V}_k = (\hat{v}_1, \ldots, \hat{v}_k) \in \mathbb{R}^{n\times k} \tag{1.4}$$

computed by the BIDIAG-2 algorithm.

In order to combine BIDIAG-1 and BIDIAG-2, the starting vector of BIDIAG-2 is chosen to be $\hat{v}_1 = v_1$ and the upper bidiagonalization of Q_L continues. It is proved in [12, 30] that the Lanczos vector $\hat{v}_i$ and the element $\hat{\beta}_i$ of $\widehat{B}_k$ can be computed by using the following relations:

$$\hat{v}_{i+1} = (-1)^i v_{i+1}, \quad \hat{\beta}_i = \alpha_{i+1}\beta_{i+1}/\hat{\alpha}_i. \tag{1.5}$$

For the large-scale matrices A and L, the explicit QR factorization (1.1) can be avoided by solving a least squares problem with $(A^T, L^T)^T$ as the coefficient matrix iteratively at each iteration [2, 21]. Through the above modifications, we obtain the JBD process which can efficiently reduce a large-scale matrix pair $\{A, L\}$ to a bidiagonal matrix pair $\{B_k, \widehat{B}_k\}$. For details of the derivation of the algorithm, see [12, 30]. In exact arithmetic, the k-step JBD process explicitly computes three-column orthonormal matrices U_{k+1}, $\widetilde{V}_k$, $\widehat{U}_k$, a lower bidiagonal matrix B_k and an upper bidiagonal matrix $\widehat{B}_k$. The two-column orthonormal matrices V_k and $\widehat{V}_k$ can be obtained from $\widetilde{V}_k$ implicitly by letting $V_k = Q^T\widehat{V}_k$ and $\widehat{V}_k = V_k P$, where $P = diag(1, -1, \ldots, (-1)^{k-1})$.

The JBD process can be used to approximate a few largest or smallest generalized singular values and corresponding vectors of $\{A, L\}$ by projecting the original large-scale problem to the reduced small-scale problem $\{B_k, \widehat{B}_k\}$. Furthermore, Kilmer et al. [12] present an iterative method based on the JBD process to solve ill-posed problems with general-form Tikhonov regularization. The main idea is to use the projection method to solve a sequence of small-scale general-form Tikhonov regularization problems which lies in lower dimensional subspaces. Jia and Yang [11] have analyzed this iterative regularized method and they present a new iterative regularized algorithm.

In exact arithmetic, the k-step JBD algorithm is equivalent to the combination of the lower and upper Lanczos bidiagonalization processes. The lower Lanczos bidiagonalization process computes two-column orthonormal matrices U_{k+1} and v_k, while the upper Lanczos bidiagonalization process computes two-column orthonormal matrices $\widehat{U}_k$ and $\widehat{V}_k$. In finite precision arithmetic, however, the orthogonality of Lanczos vectors computed by the JBD process is gradually lost, which is due to the influence of rounding errors. For the GSVD computation, the loss of orthogonality of Lanczos vectors will lead to a delay of the convergence of Ritz values and it causes the appearance of spurious generalized singular values, which are called ghosts [10, 30]. In order to preserve the convergence of the approximate generalized singular values, we need to perform the JBD process with a reorthogonalization strategy to maintain some level of orthogonality of the Lanczos vectors.

The loss of orthogonality of Lanczos vectors is a typical phenomenon appearing in the Lanczos-type algorithms, which is first observed in the symmetric Lanczos process [13]. It will lead to a delay of convergence in the computation of some extreme eigenvalues of a symmetric matrix [15–17, 19], and sometimes it is also difficult to determine whether some computed approximations are additional copies or genuine close eigenvalues [16–19]. In order to preserve the convergence, a few reorthogonalization strategies have been proposed to maintain some level of orthogonality [22–26]. Especially, Simon [26] proves that semiorthogonality of Lanczos vectors is enough to guarantee the accuracy of the computed quantities and avoid spurious eigenvalues. The above results of the symmetric Lanczos process have been adapted by Larsen to handle the Lanczos bidiagonalization process, and he proposes the Lanczos bidiagonalization with partial reorthogonalization algorithm [14], which can save a big amount of reorthogoanlization work, compared with the full reorthogonalization strategy. In [27], Simon and Zha propose a one-sided reorthogonalization strategy for the Lanczos bidiagonalization process. Later in [1], the Lanczos bidiagonalization process with the one-sided reorthogonalization has been analyzed in detail by Barlow.

In this paper, we propose a semiorthogonalization strategy for the k-step JBD process to keep the orthogonality levels of u_i, $\tilde{v}_i$, and $\hat{u}_i$ below $\sqrt{\varepsilon/(2k+1)}$, where ε is the roundoff unit. We make a rounding error analysis of the JBD process with the semiorthogonalization strategy, which establishes connections between the JBD process with the semiorthogonalization strategy and the Lanczos bidiagonalization process in finite precision arithmetic. The approximate generalized singular values of $\{A, L\}$ can be computed by using the singular value decomposition (SVD) of either B_k or $\widehat{B}_k$ [10, 30]. We will prove that semiorthogonality of the Lanczos vectors is enough to preserve convergence of the Ritz values computed from either B_k or $\widehat{B}_k$,

and the generalized singular values can be approximated with high accuracy by using the SVD of B_k, while the accuracy of the approximated generalized singular values computed from $\widehat{B}_k$ is high enough as long as $\|\widehat{B}_k^{-1}\|$ does not become too large.

Based on the semiorthogonalization strategy, we develop a practical algorithm called the joint bidiagonalization process with partial reorthogonalization (JBDPRO). The central idea in partial reorthogonalization is that the levels of orthogonality among the Lanczos vectors satisfy a coupled recurrence relations [14, 26], which can be used as a practical tool for computing estimates of the levels of orthogonality in an efficient way and to decide when to reorthogonalize, and which Lanczos vectors are necessary to be included in the reorthogonalization step. Numerical experiments show that our JBDPRO algorithm is more efficient than the joint bidiagonalization process with full reorthogonalization (JBDFRO), but can prevent "ghosts" from appearing.

This paper is organized as follows. In Section 2, we review the JBD process with some properties, and we review the GSVD computation based on the JBD process. In Section 3, we propose a semiorthogonalization strategy, and make a detailed analysis of the JBD process with the semiorthogonalization strategy. Based on the semiorthogonalization strategy, in Section 4, we develop the JBDPRO algorithm. In Section 5, we use some numerical examples to illustrate our theory and algorithm. Finally, we conclude the paper 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 zero vector of dimension k and the zero matrix of $k \times l$, respectively. The subscripts are omitted when there is no confusion. We denote by $span(C)$ the subspace spanned by columns of a matrix C. The transpose of a matrix C is denoted by C^T. The roundoff unit is denoted by ε. The norm $\|\cdot\|$ always means the spectral or 2-norm of a matrix or vector.

2 Joint bidiagonalization process and GSVD computation

In this section, we review the joint bidiagonalization process and its basic properties in both exact and finite precision arithmetic. We also describe the GSVD computation of $\{A, L\}$ based on the JBD process.

The joint bidiagonalization process is described in Algorithm 1. Notice that for the large-scale matrices A and L, the explicit QR factorization (1.1) is impractical due to efficiency and storage. At each iteration $i = 1, 2, \ldots, k+1$, Algorithm 1 needs to compute $QQ^T\begin{pmatrix} u_i \\ 0_p \end{pmatrix}$, which is not accessible since Q is not available. Let $\tilde{u}_i = \begin{pmatrix} u_i \\ 0_p \end{pmatrix}$. Notice that $QQ^T\tilde{u}_i$ is nothing but the orthogonal projection of $\tilde{u}_i$ onto the column space of $\begin{pmatrix} A \\ L \end{pmatrix}$, which means that $QQ^T\tilde{u}_i = \begin{pmatrix} A \\ L \end{pmatrix}\tilde{x}_i$, where

$$\tilde{x}_i = \arg\min_{\tilde{x}\in\mathbb{R}^n} \left\| \begin{pmatrix} A \\ L \end{pmatrix}\tilde{x} - \tilde{u}_i \right\|. \tag{2.1}$$

The large-scale least squares problem (2.1) can be solved by an iterative solver, e.g., the most commonly used LSQR algorithm [21].

Algorithm 1 The k-step joint bidiagonalization(JBD) process.

Choosing a starting vector $b \in \mathbb{R}^m$, $\beta_1 u_1 = b,\ \beta_1 = \|b\|$

$\alpha_1 \tilde{v}_1 = QQ^T \begin{pmatrix} u_1 \\ 0_p \end{pmatrix}$

$\hat{\alpha}_1 \hat{u}_1 = \tilde{v}_1(m+1 : m+p)$

for $i = 1, 2, \ldots, k$, **do**

  $\beta_{i+1} u_{i+1} = \tilde{v}_i(1 : m) - \alpha_i u_i$

  $\alpha_{i+1} \tilde{v}_{i+1} = QQ^T \begin{pmatrix} u_{i+1} \\ 0_p \end{pmatrix} - \beta_{i+1} \tilde{v}_i$

  $\hat{\beta}_i = (\alpha_{i+1}\beta_{i+1})/\hat{\alpha}_i$

  $\hat{\alpha}_{i+1} \hat{u}_{i+1} = (-1)^i \tilde{v}_{i+1}(m+1 : m+p) - \hat{\beta}_i \hat{u}_i$

end for

Algorithm 1 is actually a procedure that can be used to compute the CS decomposition of Q_A, Q_L when it is run to completion, where all we have access to is an approximation to the projection QQ^T, which can be accessed by solving (2.1) iteratively. In exact arithmetic, the k-step JBD process produces two bidiagonal matrices B_k, $\widehat{B}_k$ and three-column orthonormal matrices U_{k+1}, $\widehat{U}_k$ and

$$\widetilde{V}_k = (\tilde{v}_1, \ldots, \tilde{v}_k) \in \mathbb{R}^{(m+p)\times k} \tag{2.2}$$

satisfying $\tilde{v}_i = Q v_i$. We have $v_i = Q^T \tilde{v}_i$ and $\hat{v}_i = (-1)^{i-1} v_i$, which can be obtained implicitly from $\tilde{v}_i$. The first k steps of the recurrences from Algorithm 1 are captured in matrix form as:

$$(I_m, 0_{m\times p})\widetilde{V}_k = U_{k+1} B_k, \tag{2.3}$$

$$QQ^T \begin{pmatrix} U_{k+1} \\ 0_{p\times(k+1)} \end{pmatrix} = \widetilde{V}_k B_k^T + \alpha_{k+1} \tilde{v}_{k+1} e_{k+1}^T, \tag{2.4}$$

$$(0_{p\times m}, I_p)\widetilde{V}_k P = \widehat{U}_k \widehat{B}_k, \tag{2.5}$$

where $P = diag(1, -1, 1, \ldots, (-1)^{k-1})$, and e_{k+1} is the $(k+1)$-th column of the identity matrix of order $k+1$. In exact arithmetic, one can verify that

$$Q_A V_k = U_{k+1} B_k, \quad Q_A^T U_{k+1} = V_k B_k^T + \alpha_{k+1} v_{k+1} e_{k+1}^T, \tag{2.6}$$

$$Q_L \widehat{V}_k = \widehat{U}_k \widehat{B}_k, \quad Q_L^T \widehat{U}_k = \widehat{V}_k \widehat{B}_k^T + \hat{\beta}_k \hat{v}_{k+1} e_k^T, \tag{2.7}$$

where e_k the k-th column of the identity matrix of order k. Therefore, the JBD process of $\{A, L\}$ is equivalent to the combination of the lower and upper Lanczos bidiagonalizations of Q_A and Q_L.

The JBD process can be used to approximate some extreme generalized singular values and vectors of a large sparse or structured matrix pair $\{A, L\}$. We first describe the GSVD of $\{A, L\}$. Let

$$Q_A = P_A C_A W^T, \quad Q_L = P_L S_L W^T \tag{2.8}$$

be the CS decomposition of the matrix pair $\{Q_A, Q_L\}$ [29], where $P_A = (p_1^A, \ldots, p_m^A) \in \mathbb{R}^{m\times m}$, $P_L = (p_1^L, \ldots, p_p^L) \in \mathbb{R}^{p\times p}$ and $W = (w_1, \ldots, w_n) \in \mathbb{R}^{n\times n}$ are orthogonal matrices, and $C_A \in \mathbb{R}^{m\times n}$ and $S_L \in \mathbb{R}^{p\times n}$ are diagonal matrices (not necessarily square) satisfying $C_A^T C_A + S_L^T S_L = I_n$. Assume that the diagonals c_i of C_A are labeled in decreasing order. If we add the assumption that $(A^T, L^T)^T$ has full column rank, the GSVD of $\{A, L\}$ is

$$A = P_A C_A G^{-1}, \quad L = P_L S_L G^{-1} \tag{2.9}$$

with $G = R^{-1}W \in \mathbb{R}^{n\times n}$. Assume that the c_i are labeled in decreasing order. Then the i-th generalized singular value of $\{A, L\}$ is c_i/s_i, and the i-th corresponding generalized singular vectors are $g_i = R^{-1}w_i$, p_i^A, and p_i^L. We call g_i the i-th right generalized singular vector, p_i^A and p_i^L the i-th left generalized singular vectors corresponding to A and L, respectively. Since $c_i/s_i = \infty$ when $s_i = 0$, we use the number pair $\{c_i, s_i\}$ to denote c_i/s_i.

After the k-step JBD process of $\{A, L\}$, we have computed B_k and $\widehat{B}_k$. Let us assume that we have computed the compact SVD of B_k:

$$B_k = P_k \Theta_k W_k^T, \quad \Theta_k = diag(c_1^{(k)}, \ldots, c_k^{(k)}), \quad 1 \geq c_1^{(k)} > \cdots > c_k^{(k)} \geq 0\,, \tag{2.10}$$

where $P_k = (p_1^{(k)}, \ldots, p_k^{(k)}) \in \mathbb{R}^{(k+1)\times k}$ and $W_k = (w_1^{(k)}, \ldots, w_k^{(k)}) \in \mathbb{R}^{k\times k}$ are column orthonormal, and $\Theta_k \in \mathbb{R}^{k\times k}$. The decomposition (2.10) can be achieved by a variety of methods since B_k is a bidiagonal matrix of relatively small dimension. The approximate generalized singular value of $\{A, L\}$ is $\{c_i^{(k)}, (1-(c_i^{(k)})^2)^{1/2}\}$, while the approximate right vector is $x_i^{(k)} = R^{-1}V_k w_i^{(k)}$ and the approximate left vector corresponding to A is $y_i^{(k)} = U_{k+1}p_i^{(k)}$. For large-scale matrices A and L, the explicit computation of R^{-1} can be avoided. Notice that

$$\begin{pmatrix} A \\ L \end{pmatrix} x_i^{(k)} = QRR^{-1}V_k w_i^{(k)} = \widetilde{V}_k w_i^{(k)}.$$

Hence by solving a least squares problem, we can obtain $x_i^{(k)}$ from $\widetilde{V}_k w_i^{(k)}$. If we also want to compute the approximate left generalized singular vectors corresponding to L, we need to compute the SVD of $\widehat{B}_k$. The approximate generalized singular values and corresponding right vectors can also be computed from the SVD of $\widehat{B}_k$. The procedure is similar to the above and we omit it; for details, see [10, 30].

In finite precision arithmetic, due to rounding errors, the behavior of the JBD process will deviate far from the ideal case in exact arithmetic, and the convergence and accuracy of the approximate generalized singular values and vectors computed by using the JBD process will be affected. The rounding error analysis of the JBD process in finite precision arithmetic is based on a set of assumptions and properties of the behavior of the rounding errors occurring, which constitutes a rational model for the actual computation. We state them here, following [10].

First, we always assume that (2.1) is solved accurately at each iteration. Thus, the computed $\begin{pmatrix} A \\ L \end{pmatrix} \tilde{x}_i$ is equal to the value of $QQ^T \begin{pmatrix} u_i \\ 0_p \end{pmatrix}$ computed by explicitly using the strictly column orthonormal matrix Q. Second, the rounding errors appearing in the computation at each step are assumed to be of order $O(\varepsilon)$. Third, the property of local orthogonality of u_i and $\hat{v}_i$ holds, that is, locally the orthogonality levels of u_i and $\hat{v}_i$ satisfy the following relations respectively:

$$\beta_{i+1}|u_{i+1}^T u_i| = O(c_1(m,n)\varepsilon), \tag{2.11}$$

$$\hat{\alpha}_{i+1}|\hat{u}_{i+1}^T \hat{u}_i| = O(c_2(p,n)\varepsilon), \tag{2.12}$$

where $c_1(m,n)$ and $c_2(p,n)$ are two modestly growing functions of m, n, and p. Finally, we assume that

$$no\ \alpha_i,\ \beta_{i+1},\ \hat{\alpha}_i\ and\ \hat{\beta}_i\ ever\ become\ negligible, \tag{2.13}$$

which is almost always true in practice, and the rare cases where α_i, β_{i+1}, $\hat{\alpha}_i$, or $\hat{\beta}_i$ do become small are actually the lucky ones, since then the algorithm should be terminated, having found an approximate invariant singular subspace. Besides, we always assume that the computed Lanczos vectors are of unit length.

Under the above assumptions, it has been shown in [10] that

$$\|\widetilde{V}_k - QV_k\| = O(\|\underline{B}_k^{-1}\|\varepsilon) \tag{2.14}$$

with $\underline{B}_k = \begin{pmatrix} B_{k-1}^T \\ \alpha_k e_k^T \end{pmatrix} \in \mathbb{R}^{k\times k}$, which implies that $\widetilde{V}_k$ gradually deviates from the column space of Q as the iterations progress. Furthermore, the following four relations hold:

$$Q_A V_k = U_{k+1}B_k + F_k,\quad Q_A^T U_{k+1} = V_k B_k^T + \alpha_{k+1}v_{k+1}e_{k+1}^T + G_{k+1}, \tag{2.15}$$

$$Q_L \widehat{V}_k = \widehat{U}_k \widehat{B}_k + \widehat{F}_k,\qquad Q_L^T \widehat{U}_k = \widehat{V}_k \widehat{B}_k^T + \hat{\beta}_k \hat{v}_{k+1} e_k^T + \widehat{G}_k, \tag{2.16}$$

where

$$\|F_k\| = O(\|\underline{B}_k^{-1}\|\varepsilon),\quad \|G_{k+1}\| = O(\varepsilon), \tag{2.17}$$

$$\|\widehat{F}_k\| = O(\|\underline{B}_k^{-1}\|\varepsilon),\quad \|\widehat{G}_k\| = O((\|\underline{B}_k^{-1}\| + \|\widehat{B}_k^{-1}\|)\varepsilon). \tag{2.18}$$

Remark 2.1 The growth speed of $\|\underline{B}_k^{-1}\|$ can be controlled. In the GSVD computation problems, usually at least one matrix of $\{A, L\}$ is well conditioned, which means that at least one of $\{Q_A, Q_L\}$ is well conditioned. If Q_A is the well-conditioned one, we implement the JBD process of $\{A, L\}$, while if Q_L is the well-conditioned one, we implement the JBD process of $\{L, A\}$. By this modification, we could always make sure that $\underline{B}_k$ is a well-conditioned matrix and $\|\underline{B}_k^{-1}\|$ does not become too large.

Following Remark 2.1, we can always assume that $\|\underline{B}_k^{-1}\| = O(1)$. Thus, we can make sure that $\tilde{V}_k$ is approximately in the subspace spanned by the columns of Q within error $O(\varepsilon)$, and $\|F_k\|$, $\|\widehat{F}_k\|$ are about $O(\varepsilon)$. Therefore, (2.15) indicates that the process of computing U_{k+1}, V_k, and B_k can be treated as the lower Lanczos bidiagonalization of Q_A within error $O(\varepsilon)$. However, if $\|\widehat{B}_k^{-1}\|$ becomes too large,

the process of computing $\widehat{U}_k$, $\widehat{V}_k$, and $\widehat{B}_k$ will deviate far from the upper Lanczos bidiagonalization of Q_L.

In finite precision arithmetic, the Lanczos vectors computed by the JBD process gradually lose their mutual orthogonality as the iteration number k increases. Following [10], we give the definition of the orthogonality level of a group of vectors.

Definition 2.1 For a rectangular matrix $W_k = (w_1, \ldots, w_k) \in \mathbb{R}^{r\times k}$ with $\|w_j\| = 1$, $j = 1, \ldots, k$, two measures of the orthogonality level of $\{w_1, \ldots, w_k\}$ or W_k are:

$$\kappa(W_k) = \max_{1\le i\ne j\le k} |w_i^T w_j|, \quad \xi(W_k) = \|I_k - W_k^T W_k\|.$$

In the following analysis, we often use terminology "the orthogonality level of w_i" for simplicity, which means the orthogonality level of $\{w_1, \ldots, w_k\}$. Notice that $\kappa(W_k) \le \xi(W_k) \le k\kappa(W_k)$. In most occasions, the two quantities can be used interchangeably to measure the orthogonality level of Lanczos vectors. We call w_i "semiorthogonal" if its orthogonality level is about $\sqrt{\varepsilon}$. Using the method in [1], we can obtain $\|W_k\| \le \sqrt{1 + \xi(W_k)}$. This upper bound will be used later.

If we use the JBD process to approximate some generalized singular values and vectors of $\{A, L\}$, the loss of orthogonality of Lanczos vectors will lead to a delay of the convergence of approximate generalized singular values and the appearance of "ghosts." To preserve the convergence, one can use the full reorthogonalization for u_i, $\hat{u}_i$, and $\tilde{v}_i$ at each iteration, to make sure that the orthogonality levels of u_i, $\hat{u}_i$, and $\tilde{v}_i$ are about $O(\varepsilon)$. The disadvantage of full reorthogonalization strategy is that it will cost too much extra computation. It has been shown in [10] that semiorthogonality of Lanczos vectors is enough to guarantee the accuracy of the approximate generalized singular values and prevent ghosts from appearing. In the next section, we will propose a semiorthogonalization strategy, and make a detailed analysis of the JBD process equipped with the semiorthogonalization strategy.

3 A semiorthogonalization strategy for the JBD process

Now we introduce a semiorthogonalization strategy for the JBD process. The semiorthogonalization strategy is similar to that proposed by Simon for the symmetric Lanczos process [26]. We use the reorthogonalization of u_{i+1} to describe it. Let $\omega_0 = \sqrt{\varepsilon/(2k+1)}$. At the i-th step, suppose that

$$\beta'_{i+1}u'_{i+1} = \tilde{v}_i(1:m) - \alpha_i u_i - f'_i.$$

If $|u'^T_{i+1}u_j| > \omega_0$ for some $j < i$, then we choose $i-1$ real numbers $\xi_{1i}, \ldots, \xi_{i-1,i}$, and form

$$\beta_{i+1}u_{i+1} = \beta'_{i+1}u'_{i+1} - \sum_{j=1}^{i-1}\xi_{ji}u_j - f''_i.$$

In the above equations, f'_i and f''_i are rounding error terms in the computation. The algorithm will be continued with u_{i+1} instead of u'_{i+1}.

Definition 3.1 The above modification of the JBD process will be called a semiorthogonalization stategy for u_{i+1} if the following conditions are satisfied:

1. The numbers $\xi_{1i}, \ldots, \xi_{i-1,i}$ are chosen such that
$$\left| u_{i+1}^T u_j \right| \le \omega_0 \,, \quad j = 1, \ldots, i. \tag{3.1}$$
2. The computation of u_{i+1} can be written as
$$\beta_{i+1} u_{i+1} = \tilde{v}_i(1:m) - \alpha_i u_i - \sum_{j=1}^{i-1} \xi_{ji} u_j - f_i, \tag{3.2}$$
where $f_i = f_i' + f_i''$ is the rounding error term and satisfies $\|f_i\| = O(q_1(m,n)\varepsilon)$ with $q_1(m,n)$ a modestly growing function of m and n.

The semiorthogonalization stategies for $\tilde{v}_{i+1}$ and $\hat{u}_{i+1}$ are similar, and the corresponding i-th step recurrences are

$$\alpha_{i+1}\tilde{v}_{i+1} = QQ^T \begin{pmatrix} u_{i+1} \\ 0_p \end{pmatrix} - \beta_{i+1}\tilde{v}_i - \sum_{j=1}^{i-1} \eta_{ji+1}\tilde{v}_j - g_{i+1}, \tag{3.3}$$

$$\hat{\alpha}_{i+1}\hat{u}_{i+1} = (-1)^i \tilde{v}_{i+1}(m+1:m+p) - \hat{\beta}_i \hat{u}_i - \sum_{j=1}^{i-1} \hat{\xi}_{ji+1}\hat{u}_j - \hat{f}_{i+1}, \tag{3.4}$$

where $\|g_{i+1}\| = O(q_2(m,p)\varepsilon)$ and $\|\hat{f}_{i+1}\| = O(q_3(p,n)\varepsilon)$ with $q_2(m,p)$ and $q_3(p,n)$ two modestly growing functions of m, n, and p.

Notice that the reorthogonalization of u_{i+1} does not use the vector u_i, due to the property of local orthogonality among u_i and u_{i+1}. The reasons are similar for the reorthogonalizations of $\tilde{v}_{i+1}$ and $\hat{u}_{i+1}$. After the semiorthogonalization step, relations (2.11) and (2.12) will still hold.

After k steps, we have computed three groups of Lanczos vectors $\{u_1, \ldots, u_{k+1}\}$, $\{\tilde{v}_1, \ldots, \tilde{v}_k\}$ and $\{\hat{u}_1, \ldots, \hat{u}_k\}$, whose orthogonality levels are below ω_0. The first k steps of the recurrences are captured in matrix form as

$$(I_m, 0_{m\times p})\widetilde{V}_k = U_{k+1}(B_k + C_k) + \widehat{F}_k, \tag{3.5}$$

$$QQ^T \begin{pmatrix} U_{k+1} \\ 0_{p\times(k+1)} \end{pmatrix} = \widetilde{V}_k(B_k^T + D_k) + \alpha_{k+1}\tilde{v}_{k+1}e_{k+1}^T + \widehat{G}_{k+1}, \tag{3.6}$$

$$(0_{p\times m}, I_p)\widetilde{V}_k P = \widehat{U}_k(\widehat{B}_k + \widehat{C}_k) + \bar{F}_k, \tag{3.7}$$

where $\widetilde{F}_k = (f_1, \ldots, f_k)$, $\widetilde{G}_{k+1} = (g_1, \ldots, g_{k+1})$, $\bar{F}_k = (\hat{f}_1, \ldots, \hat{f}_k)$, and

$$C_k = \begin{pmatrix} 0 & \xi_{12} & \cdots & \xi_{1k} \\ 0 & 0 & \cdots & \xi_{2k} \\ & 0 & \ddots & \vdots \\ & & \ddots & 0 \\ & & & 0 \end{pmatrix} \in \mathbb{R}^{(k+1)\times k}, \quad \widehat{C}_k = \begin{pmatrix} 0 & 0 & \hat{\xi}_{13} & \cdots & \hat{\xi}_{1k} \\ & 0 & 0 & \cdots & \hat{\xi}_{2k} \\ & & \ddots & \ddots & \vdots \\ & & & 0 & 0 \\ & & & & 0 \end{pmatrix} \in \mathbb{R}^{k\times k},$$

$$D_k = \begin{pmatrix} 0 & 0 & \eta_{13} & \cdots & \eta_{1k} & \eta_{1k+1} \\ & 0 & 0 & \eta_{24} & \cdots & \eta_{2k+1} \\ & & \ddots & \ddots & \ddots & \vdots \\ & & & \ddots & 0 & \eta_{k-1,k+1} \\ & & & & 0 & 0 \end{pmatrix} \in \mathbb{R}^{k\times(k+1)}.$$

Notice that the columns $\tilde{v}_i$ of $\tilde{V}_k$ are approximately in the subspace spanned by the columns of Q within error $O(\varepsilon)$ for $i = 1, \ldots, k$. If we let $\nu_i = Q^T\tilde{v}_i$ and $\hat{v}_i = (-1)^{i-1}\nu_i$, then $\widetilde{V}_k = QV_k + O(\varepsilon)$, and $\{\nu_1, \ldots, \nu_k\}$ and $\{\hat{v}_1, \ldots, \hat{v}_k\}$ are also kept semiorthogonal. From (3.5)–(3.7), we can obtain

$$Q_A V_k = U_{k+1}(B_k + C_k) + F_k, \tag{3.8}$$

$$Q_A^T U_{k+1} = V_k(B_k^T + D_k) + \alpha_{k+1}v_{k+1}e_{k+1}^T + G_{k+1}, \tag{3.9}$$

$$Q_L \widehat{V}_k = \widehat{U}_k(\widehat{B}_k + \widehat{C}_k) + \widehat{F}_k, \tag{3.10}$$

where $\|F_k\| = O(q_1(m,n)\varepsilon)$, $\|G_{k+1}\| = O(q_2(m,p)\varepsilon)$, and $\|\widehat{F}_k\| = O(q_3(p,n)\varepsilon)$. We point out that the rounding error terms F_k, G_{k+1}, and $\widehat{F}_k$ here are different from those in relations (2.15)–(2.18), and we use the same notations just for simplicity.

The following two lemmas describe some basic properties of the JBD process with the semiorthogonalization strategy. The proofs are given in Appendix 1.

Lemma 3.1 *For the k-step JBD process with the semiorthogonalization strategy, the relation*

$$Q_L^T\hat{u}_i \in span\{\hat{v}_1, \ldots, \hat{v}_{i+1}\} + O(\bar{q}(m,n,p)\varepsilon). \tag{3.11}$$

holds for all $i = 1, 2, \ldots, k$ *where* $\bar{q}(m,n,p) = q_1(m,n) + q_2(m,p) + q_3(p,n)$.

Lemma 3.2 *For the k-step JBD process with the semiorthogonalization strategy, we have*

$$C_k = O(\sqrt{\varepsilon}), \quad D_k = O(\sqrt{\varepsilon}), \quad \widehat{C}_k = O(\sqrt{\varepsilon}), \tag{3.12}$$

where $X = O(\sqrt{\varepsilon})$ *for a matrix X means that all the elements of X are of* $O(\sqrt{\varepsilon})$.

Now, we give a relation between the two computed quantities B_k and $\widehat{B}_k$.

Theorem 3.1 *Given the k-step JBD process with the semiorthogonalization strategy, we have*

$$B_k^T B_k + P\widehat{B}_k^T\widehat{B}_k P = I_k + H_k, \tag{3.13}$$

where H_k *is a symmetric tridiagonal matrix the "symmetric tridiagonal matrix" has already meant that its bandwidth is 1, and the nonzero elements of* H_k *are of* $O(c_3(m,n,p)\varepsilon)$ *with* $c_3(m,n,p) = c_1(m,n) + c_2(p,n) + q_1(m,n) + q_3(p,n)$.

Proof Since

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

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

nonzero elements in H_k are contained only in the diagonal and subdiagonal parts.

For their diagonal parts, from (3.2) we have

$$\begin{aligned} \|\tilde{u}_i(1:m)\|^2 &= \|\alpha_i u_i + \beta_{i+1}u_{i+1} + \sum_{j=1}^{i-1}\xi_{ji}u_j + f_i\|^2 \\ &= \alpha_i^2 + \beta_{i+1}^2 + 2\alpha_i\beta_{i+1}u_i^T u_{i+1} + 2\alpha_i u_i^T f_i + 2\beta_{i+1}u_{i+1}^T f_i + \|f_i\|^2 \\ &\quad + \|\sum_{j=1}^{i-1}\xi_{ji}u_j\|^2 + 2\alpha_i\sum_{j=1}^{i-1}\xi_{ji}u_i^T u_j + 2\beta_{i+1}\sum_{j=1}^{i-1}\xi_{ji}u_{i+1}^T u_j \\ &\quad + 2\sum_{j=1}^{i-1}\xi_{ji}f_i^T u_j. \end{aligned}$$

Since $\xi_{ji} = O(\sqrt{\varepsilon})$ and $\left|u_l^T u_j\right| \le \sqrt{\varepsilon/(2k+1)}$ for $1 \le l \ne j \le i+1$, we obtain

$$\begin{aligned} &\|\sum_{j=1}^{i-1}\xi_{ji}u_j\|^2 + 2\alpha_i\sum_{j=1}^{i-1}\xi_{ji}u_i^T u_j + 2\beta_{i+1}\sum_{j=1}^{i-1}\xi_{ji}u_{i+1}^T u_j + 2\sum_{j=1}^{i-1}\xi_{ji}f_i^T u_j \\ =\ & 2\sum_{1\le j<l\le i-1}\xi_{ji}\xi_{li}u_j^T u_l + \sum_{j=1}^{i-1}\xi_{ji}^2\|u_j\|^2 + 2\alpha_i\sum_{j=1}^{i-1}O(\varepsilon) + 2\beta_{i+1}\sum_{j=1}^{i-1}O(\varepsilon) \\ &+ 2\sum_{j=1}^{i-1}O(\varepsilon\sqrt{\varepsilon}) \\ =\ & O(i\varepsilon\sqrt{\varepsilon}) + O(i\varepsilon) + O[i(\alpha_i+\beta_{i+1})\varepsilon] + O(i\varepsilon\sqrt{\varepsilon}) \\ =\ & O(i\varepsilon). \end{aligned}$$

Using the property of local orthogonality of u_i , we have

$$2\alpha_i\beta_{i+1}u_i^T u_{i+1} + 2\alpha_i u_i^T f_i + 2\beta_{i+1}u_{i+1}^T f_i + \|f_i\|^2 = O(\bar{c}_1(m,n)\varepsilon)$$

with $\bar{c}_1(m,n) = c_1(m,n) + q_1(m,n)$. Thus

$$\|\tilde{v}_i(1:m)\|^2 = \alpha_i^2 + \beta_{i+1}^2 + O(\bar{c}_1(m,n)\varepsilon).$$

Similarly, from (3.4), we can obtain

$$\|\tilde{v}_i(m+1:m+p)\|^2 = \hat{\alpha}_i^2 + \hat{\beta}_{i-1}^2 + O(\bar{c}_2(p,n)\varepsilon)$$

with $\bar{c}_2(p,n) = c_2(p,n) + q_3(p,n)$. Since

$$1 = \|\tilde{v}_i\|^2 = \|\tilde{v}_i(1:m)\|^2 + \|\tilde{u}_i(m+1:m+p)\|^2,$$

we get

$$\alpha_i^2 + \beta_{i+1}^2 + \hat{\alpha}_i^2 + \hat{\beta}_{i-1}^2 = 1 + O(c_3(m,n,p)\varepsilon). \tag{3.14}$$

For the subdiagonal parts, in finite precision arithmetic, we have $\hat{\beta}_i = (\alpha_{i+1}\beta_{i+1}/\hat{\alpha}_i)\,(1+\tau)$, where $|\tau| \le \varepsilon$ [9, §2.2], showing that

$$\alpha_{i+1}\beta_{i+1} = \hat{\alpha}_i\hat{\beta}_i - \alpha_{i+1}\beta_{i+1}\tau.$$

From (3.14), we have

$$\alpha_{i+1}\beta_{i+1} \le \frac{\alpha_{i+1}^2 + \beta_{i+1}^2}{2} \le \frac{2[1 + O(c_3(m,n,p)\varepsilon)]}{2} = 1 + O(c_3(m,n,p)\varepsilon).$$

Therefore, we obtain

$$\alpha_{i+1}\beta_{i+1} = \hat{\alpha}_i\hat{\beta}_i + \gamma_i, \tag{3.15}$$

where $|\gamma_i| \le [1 + O(c_3(m,n,p)\varepsilon)]\varepsilon = O(\varepsilon)$.

Combining (3.14) and (3.15), we finally obtain (3.13). □

We now show the connection between the process of computing $\widehat{U}_k$, $\widehat{V}_k$, $\widehat{B}_k$, and the upper Lanczos bidiagonalization of Q_L in finite precision arithmetic.

Theorem 3.2 *For the k-step JBD process with the semiorthogonalization strategy, the following relation holds:*

$$Q_L^T\widehat{U}_k = \widehat{V}_k(\widehat{B}_k^T + \widehat{D}_k) + \hat{\beta}_k\hat{v}_{k+1}e_k^T + \widehat{G}_k, \tag{3.16}$$

where $\widehat{D}_k$ is upper triangular with zero diagonals, and

$$\|\widehat{G}_k\| = O(c_4(m,n,p)\|\widehat{B}_k^{-1}\|\varepsilon), \tag{3.17}$$

with $c_4(m,n,p) = c_1(m,n) + c_2(p,n) + \bar{q}(m,n,p)$.

Proof Combining (3.8) and (3.9), we have

$$\begin{aligned} Q_A^T Q_A V_k &= Q_A^T U_{k+1}(B_k + C_k) + Q_A^T F_k \\ &= [V_k(B_k^T + D_k) + \alpha_{k+1}v_{k+1}e_{k+1}^T + G_{k+1}](B_k + C_k) + Q_A^T F_k \\ &= V_k B_k^T B_k + \alpha_{k+1}\beta_{k+1}v_{k+1}e_k^T + V_k(B_k^T + D_k)C_k + V_k D_k B_k + \\ &\qquad G_{k+1}(B_k + C_k) + Q_A^T F_k. \end{aligned}$$

Premultiplying (3.10) by Q_L^T, we have

$$Q_L^T Q_L V_k = [Q_L^T\widehat{U}_k(\widehat{B}_k + \widehat{C}_k) + Q_L^T\widehat{F}_k]P.$$

Adding the above two equalities, we obtain

$$\begin{aligned}&(Q_A^T Q_A + Q_L^T Q_L)V_k\\ =\ & V_k[I_k - P\widehat{B}_k^T\widehat{B}_k P + H_k] + Q_L\widehat{U}_k\widehat{B}_k^T P + (\hat{\alpha}_k\hat{\beta}_k + \gamma_k)v_{k+1}e_k^T + V_k D_k B_k\\ & + V_k(B_k^T + D_k)C_k + Q_L^T\widehat{U}_k\widehat{C}_k P + G_{k+1}(B_k + C_k) + Q_A^T F_k + Q_L^T\widehat{F}_k P.\end{aligned}$$

Since $(Q_A^T Q_A + Q_L^T Q_L)V_k = V_k$, after some rearrangement we obtain

$$\widehat{V}_k\widehat{B}_k^T\widehat{B}_k = Q_L^T\widehat{U}_k\widehat{B}_k - \hat{\alpha}_k\hat{\beta}_k\hat{v}_{k+1}e_k^T + \bar{E}_1 + \bar{E}_2,$$

where

$$\bar{E}_1 = \widehat{V}_k P[D_k B_k + (B_k^T + D_k)C_k]P + Q_L^T\widehat{U}_k\widehat{C}_k,$$

and

$$\bar{E}_2 = [G_{k+1}(B_k + C_k) + Q_A^T F_k + Q_L^T\widehat{F}_k P + V_k H_k]P - \gamma_k\hat{v}_{k+1}e_k^T.$$

According to the structure of matrices C_k and D_k, by a simple calculation, we can verify that $P[D_k B_k + (B_k^T + D_k)C_k]P$ is an upper triangular matrix with zero diagonals, which is denoted by Y_k. Notice that the i-th column of $Q_L^T\widehat{U}_k\widehat{C}_k$ is $\sum_{j=1}^{i-2}\hat{\xi}_{ji}Q_L^T\hat{u}_j$. By Lemma 3.1, there exist coefficients $\rho_{1i}, \ldots, \rho_{i-1,i}$ such that

$$\sum_{j=1}^{i-2}\hat{\xi}_{ji}Q_L^T\hat{u}_j = \sum_{j=1}^{i-1}\rho_{ji}\hat{v}_j + O(\bar{q}(m, n, p)\varepsilon).$$

Therefore, we have

$$Q_L^T\widehat{U}_k C_k = \widehat{V}_k W_k + O(\bar{q}(m, n, p)\varepsilon),$$

where

$$W_k = \begin{pmatrix} 0 & \rho_{12} & \rho_{13} & \cdots & \rho_{1k}\\ & 0 & \rho_{23} & \cdots & \rho_{2k}\\ & & \ddots & \ddots & \vdots\\ & & & \ddots & \rho_{k-1,k}\\ & & & & 0\end{pmatrix} \in \mathbb{R}^{k\times k}$$

is upper triangular with zero diagonals.

Notice that $\|V_k\| \le \sqrt{1 + \xi(V_k)} = 1 + O(\sqrt{\varepsilon})$. From (3.14), we can get[1]

$$\|B_k\| \le \sqrt{2}\max_{1\le i\le k}(\alpha_i^2 + \beta_{i+1}^2)^{1/2} \le \sqrt{2} + O(c_3(m, n, p)\varepsilon).$$

By Theorem 3.1, we can get

$$\|H_k\| = O(c_3(m, n, p)). \tag{3.18}$$

Using these upper bounds, by a simple but tedious calculation, we can prove that

$$\|\bar{E}_2\| = O(c_4(m, n, p)\varepsilon).$$

[1]Here, we use the result of an exercise from Higham's book [9, Chapter 6, Problems 6.14], which gives the upper bound of the p-norm of a row/column sparse matrix.

From the above, we obtain

$$Q_L^T \widehat{U}_k - \widehat{V}_k \widehat{B}_k^T - \hat{\beta}_k \hat{v}_{k+1} e_k^T = -\widehat{V}_k (W_k + Y_k)\widehat{B}_k^{-1} - [\bar{E}_2 + O(\bar{q}(m,n,p)\varepsilon)]\widehat{B}_k^{-1}.$$

Noticing that $-(W_k + Y_k)\widehat{B}_k^{-1}$ is upper triangular with zero diagonals, which is denoted by $\widehat{D}_k$, we finally obtain

$$Q_L^T \widehat{U}_k = \widehat{V}_k (\widehat{B}_k^T + \widehat{D}_k) + \hat{\beta}_k \hat{v}_{k+1} e_k^T + \widehat{G}_k,$$

where $\widehat{G}_k = -[\bar{E}_2 + O(\bar{q}(m,n,p)\varepsilon)]\widehat{B}_k^{-1}$ and $\|\widehat{G}_k\| = O(c_4(m,n,p)\|\widehat{B}_k^{-1}\|\varepsilon)$. □

If we write the matrix $\widehat{D}_k$ as

$$\widehat{D}_k = \begin{pmatrix} 0 & \hat{\eta}_{12} & \hat{\eta}_{13} & \cdots & \hat{\eta}_{1k} \\ & 0 & \hat{\eta}_{23} & \cdots & \hat{\eta}_{2k} \\ & & \ddots & \ddots & \vdots \\ & & & 0 & \hat{\eta}_{k-1,k} \\ & & & & 0 \end{pmatrix} \in \mathbb{R}^{k\times k},$$

then for each $i = 1, \ldots, k$, from (3.16) we have

$$\hat{\beta}_i \hat{v}_{i+1} = Q_L^T \hat{u}_i - \hat{\alpha}_i \hat{v}_i - \sum_{j=1}^{i-1} \hat{\eta}_{ji} \hat{v}_j - \hat{g}_i,$$

where $\|\hat{g}_i\| = O(c_4(m,n,p)\|\widehat{B}_k^{-1}\|\varepsilon)$, which corresponds to the reorthogonalization of $\hat{v}_i$ with the error term $\hat{g}_i$. Therefore, combining (3.10) and (3.16), we can treat the process of computing $\widehat{U}_k$, $\widehat{V}_k$, and $\widehat{B}_k$ as the upper Lanczos bidiagonalization of Q_L with the semiorthogonalization strategy within error $\delta = O(c_4(m,n,p)\|\widehat{B}_k^{-1}\|\varepsilon)$.

By (3.8) and (3.9), we can treat the process of computing U_{k+1}, V_k, and B_k as the lower Lanczos bidiagonalization of Q_A with the semiorthogonalization strategy. Therefore, the computed B_k is, up to roundoff, the Ritz-Galerkin projection of Q_A on the subspace $span(U_{k+1})$ and $span(V_k)$, i.e., we have the following result.

Theorem 3.3 *For the k-step JBD process with the semiorthogonalization strategy, suppose that the compact QR factorizations of U_k and V_k are $U_k = M_k R_k$ and $V_k = N_k S_k$, where the diagonals of the upper triangular matrices R_k and S_k are nonnegative. Then*

$$M_k^T Q_A N_k = B_k + E_k, \tag{3.19}$$

where the elements of E_k are of $O(\tilde{q}(m,n,p)\varepsilon)$ with $\tilde{q}(m,n,p) = q_1(m,n) + q_2(p,n)$.

Since the k-step Lanczos bidiagonalization is equivalent to the $(2k+1)$-step symmetric Lanczos process [2, Sect. 7.6.1], using the method in [2, Sect. 7.6.1], we can deduce Theorem 3.3 from [26, Theorem 5]. By the Wielandt-Hoffman theorem [5, Theorem 8.6.4], the singular values of B_k are, up to error $O(\tilde{q}(m,n,p)\varepsilon)$, the singular values of $M_k^T Q_A N_k$. Therefore, Theorem 3.3 means that if we use the SVD of B_k to approximate some generalized singular values of $\{A, L\}$, the singular values of B_k are identical to those ones of the true projection matrix within the level of machine precision.

In [30], the author suggests that one can also use the SVD of $\widehat{B}_k$ to approximate some generalized singular values and vectors of $\{A, L\}$. Similar to the above theorem, combining (3.10) and (3.16), we can obtain the following result.

Theorem 3.4 *For the k-step JBD process with the semiorthogonalization strategy, suppose that the compact QR factorizations of $\widehat{U}_k$ and $\widehat{V}_k$ are $\widehat{U}_k = \widehat{M}_k \widehat{R}_k$ and $\widehat{V}_k = \widehat{N}_k \widehat{S}_k$, where the diagonals of the upper triangular matrices $\widehat{R}_k$ and $\widehat{S}_k$ are nonnegative. Then*

$$\widehat{M}_k^T Q_L \widehat{N}_k = \widehat{B}_k + \widehat{E}_k, \tag{3.20}$$

where the elements of $\widehat{E}_k$ are of $\delta = O(c_4(m, n, p)\|\widehat{B}_k^{-1}\|\varepsilon)$.

Theorem 3.4 indicates that the computed $\widehat{B}_k$ equals to the Ritz-Galerkin projection of Q_L on the subspace $span(\widehat{U}_k)$ and $span(\widehat{V}_k)$ with the error $O(\delta)$. Therefore, if we use the SVD of $\widehat{B}_k$ to approximate some generalized singular values $\{A, L\}$, the singular values of $\widehat{B}_k$ are identical to those ones of the true projection matrix within the level of O(δ), which is not far from machine precision, as long as $\|\widehat{B}_k^{-1}\|$ does not become too large.

4 The JBD process with partial reorthogonalization

In order to implement the semiorthogonalization strategy, we need to decide when to reorthogonalize, and which Lanczos vectors are necessary to be included in the reorthogonalization step. By the analysis in the previous section, the process of computing U_{k+1}, V_k, and B_k can be treated as the lower Lanczos bidiagonalization of Q_A, so our reorthogonalization strategy can be based on the partial reorthogonalization of u_i and v_i; see [14, 25]. The central idea is that the levels of orthogonality of u_i and v_i satisfy the following coupled recurrences [14, Theorem 6].

Theorem 4.1 *Let $\mu_{ji} = u_j^T u_i$, $\nu_{ji} = v_j^T v_i$, and $\mu_{j0} \equiv 0$, $\nu_{j0} \equiv 0$. Then $\mu_{jj} = 1$ for $1 \le j \le i+1$ and $\nu_{jj} = 1$ for $1 \le j \le i$, and*

$$\beta_{i+1}\mu_{j,i+1} = \alpha_j \nu_{ji} + \beta_j \nu_{j-1,i} - \alpha_i \mu_{ji} - u_j^T f_i + v_i^T g_j \tag{4.1}$$

for $1 \le j \le i$ and

$$\alpha_i \nu_{ji} = \beta_{j+1}\mu_{j+1,i} + \alpha_j \mu_{ji} - \beta_i \nu_{j,i-1} + u_i^T f_j - v_j^T g_i \tag{4.2}$$

for $1 \le j \le i-1$.

Theorem 4.1 shows that the inner products $u_j^T u_{i+1}$ and $v_j^T v_i$ are simply linear combinations of the inner products formed by the previous Lanczos vectors. Thus, we can estimate quantities $\mu_{j,i+1}$ and ν_{ji} if we have proper estimations of $|u_i^T f_j - v_j^T g_i|$ and $|u_j^T f_i - v_i^T g_j|$. The two quantities $|u_i^T f_j - v_j^T g_i|$ and $|u_j^T f_i - v_i^T g_j|$ are about $O(\varepsilon)$ and their accurate estimates have been discussed in detail in [14]. Since $\tilde{v}_i^T \tilde{v}_j \approx v_i^T v_j$, the estimated ν_{ji} is also a good estimate of $\tilde{v}_j^T \tilde{v}_i$. Therefore, using these estimates, we can monitor the loss of orthogonality of Lanczos vectors u_i and

$\tilde{\nu}_i$ directly without forming inner products, which enables us to determine when and against which of the previous Lanczos vectors to reorthogonalize.

On the other hand, it has been shown in [10] that the orthogonality level of $\widehat{U}_k$ is affected not only by those of U_{k+1} and $\widetilde{V}_k$, but also by a factor $\|\widehat{B}_k^{-1}\|$. Therefore, if $\widehat{B}_k$ is not very ill-conditioned, the orthogonality of $\widehat{U}_k$ will not be too bad even if we only reorthogonalize u_i and $\tilde{\nu}_i$ but not $\hat{u}_i$. From the above discussions, we finally obtain the JBD process with partial reorthogonalization, which is described in Algorithm 2.

Algorithm 2 The k-step JBDPRO.

Choosing a starting vector $b \in \mathbb{R}^m$, $\beta_1 u_1 = b,\ \beta_1 = \|b\|$
$\alpha_1 \tilde{\nu}_1 = QQ^T \begin{pmatrix} u_1 \\ 0_p \end{pmatrix}$
$\hat{\alpha}_1 \hat{u}_1 = \tilde{\nu}_1(m+1 : m+p)$
for $i = 1, 2, \ldots, k$, **do**
    $r_{i+1} = \tilde{\nu}_i(1 : m) - \alpha_i u_i$
    Update $\mu_{ji} \to \mu_{ji+1},\ j = 1, \cdots, i$
    Determine a set of indices $T_i \subseteq \{j | 1 \le j \le i-1\}$
    for $j \in T_i$ **do**
        $r_{i+1} = r_i - (u_j^T r_{i+1}) u_j$
        Reset $\mu_{j,i+1}$ to $O(\epsilon)$
    end for
    $\beta_{i+1} u_{i+1} = r_{i+1}$
    $p_{i+1} = QQ^T \begin{pmatrix} u_{i+1} \\ 0_p \end{pmatrix} - \beta_{i+1} \tilde{\nu}_i$
    Update $\nu_{ji} \to \nu_{ji+1},\ j = 1, \cdots, i$
    Determine a set of indices $S_i \subseteq \{j | 1 \le j \le i-1\}$
    for $j \in S_i$ **do**
        $p_{i+1} = p_{i+1} - (\nu_j^T p_{i+1}) \nu_j$
        Reset $\nu_{j,i+1}$ to $O(\epsilon)$
    end for
    $\alpha_{i+1} \tilde{\nu}_{i+1} = p_i$
    $\hat{\beta} = (\alpha_{i+1} \beta_{i+1}) / \hat{\alpha}_i$
    $\hat{\alpha}_{i+1} \hat{u}_{i+1} = (-1)^i \tilde{\nu}_{i+1}(m+1 : m+p) - \hat{\beta}_i \hat{u}_i$
end for

In Algorithm 2, we need to determine two sets T_i and S_i at each iteration. The methods of choosing which previous Lanczos vectors to reorthogonalize have been discussed in detail by Simon [25] and Larsen [14], for the symmetric Lanczos process and Lanczos bidiagonalization, respectively. They introduce the η-criterion. Here, we use the reorthogonalization of u_{i+1} to explain it. At the i-th iteration, we only need to reorthogonalize against the vectors where μ_{ji+1} is larger than some constant η satisfying $\varepsilon < \eta < \omega_0$. It is sufficient to choose the vectors where μ_{ji+1} exceeds ω_0 and their neighbors exceed η to be included in the reorthogonalization step, while a

few isolated components that exceeding η are quite harmless [14, 25]. Therefore, the index sets T_i and S_i can be described by the formulas:

$$T_i = \bigcup_{\mu_{j,i+1}>\omega_0} \{l | 1 \le j-r \le l \le j+s \le i-1, \mu_{li+1} > \eta\}, \tag{4.3}$$

$$S_i = \bigcup_{\nu_{j,i+1}>\omega_0} \{l | 1 \le j-r \le l \le j+s \le i-1, \nu_{li+1} > \eta\}. \tag{4.4}$$

Simon [25] demonstrates that using the η-criterion in partial reorthogonalization could significantly reduce the amount of extra reorthogonalization work. Experimentally, he finds that $\eta = \varepsilon^{3/4}$ is the value that minimizes the total amount of reorthogonalization work for the symmetric Lanczos process. In Algorithm 2, we also choose $\eta = \varepsilon^{3/4}$ to implement the partial reorthogonalization.

For the JBDPRO algorithm with the η-criterion, the orthogonality levels of u_i and $\tilde{v}_i$ will be $O(\eta)$. By using the same method as in the proof of Lemma 3.2, we can prove that $D_k = O(\eta)$ and $C_k = O(\eta)$. Notice that we do not reorthogonalize $\hat{v}_i$, which can save a big amount of reorthogonalization work. The following theorem states that if $\widehat{B}_k$ is not very ill-conditioned, then the orthogonality of $\widehat{U}_k$ will be at a desired level.

Theorem 4.2 *For the k-step JBDPRO algorithm, the orthogonality level of* $\widehat{U}_k$ *satisfies*

$$\xi(\widehat{U}_k) = O(\|\widehat{B}_k^{-1}\|^2 \eta). \tag{4.5}$$

Proof Since we do not reorthogonalize any $\hat{v}_i$, which means that $\widehat{C}_k = 0$, by (3.10) we have

$$\widehat{B}_k^T \widehat{U}_k^T \widehat{U}_k \widehat{B}_k = (Q_L \widehat{v}_k - \widehat{F}_k)^T (Q_L \widehat{v}_k - \widehat{F}_k),$$

and

$$\begin{aligned} &\widehat{B}_k^T (I_k - \widehat{U}_k^T \widehat{U}_k) \widehat{B}_k = \widehat{B}_k^T \widehat{B}_k - (Q_L \widehat{V}_k - \widehat{F})^T (Q_L \widehat{V}_k - \widehat{F}_k) \\ &= I_k - P B_k^T B_k P + H_k - \widehat{V}_k^T Q_L^T Q_L \widehat{V}_k + \widehat{V}_k^T Q_L^T \widehat{F}_k + \widehat{F}_k^T Q_L \widehat{V}_k - \widehat{F}_k^T \widehat{F}_k \\ &= I_k - P B_k^T B_k P - P V_k^T (I_k - Q_A^T Q_A) V_k P + \widehat{V}_k^T Q_L^T \widehat{F}_k + \widehat{F}_k^T Q_L \widehat{V}_k - \widehat{F}_k^T \widehat{F}_k + H_k. \end{aligned} \tag{4.6}$$

By (3.8), we have

$$\begin{aligned} V_k^T Q_A^T Q_A V_k &= [U_{k+1}(B_k + D_k) + F_k]^T [U_{k+1}(B_k + D_k) + F_k] \\ &= B_k^T U_{k+1}^T U_{k+1} B_k + \bar{E}_3, \end{aligned} \tag{4.7}$$

where

$$\begin{aligned} \bar{E}_3 = {} & D_k^T U_{k+1}^T U_{k+1} B_k + B_k^T U_{k+1}^T U_{k+1} D_k + (B_k + D_k)^T U_{k+1}^T F_k + \\ & F_k^T U_{k+1}(B_k + D_k) + D_k^T U_{k+1}^T U_{k+1} D_k + F_k^T F_k. \end{aligned}$$

Since $D_k = O(\eta)$, by a simple calculation, we can obtain

$$\|\bar{E}_3\| = O(\eta).$$

Substituting (4.7) into (4.6), we have

$$\begin{aligned} \widehat{B}_k^T (I_k - \widehat{U}_k^T \widehat{U}_k) \widehat{B}_k = {} & (I_k - \widehat{V}_k^T \widehat{V}_k) - P B_k^T (I_{k+1} - U_{k+1}^T U_{k+1}) B_k P + \\ & \widehat{V}_k^T Q_L^T \widehat{F}_k + \widehat{F}_k^T Q_L \widehat{V}_k - \widehat{F}_k^T \widehat{F}_k + H_k + P \bar{E}_3 P. \end{aligned}$$

By a simple manipulation, we can obtain

$$\|\widehat{V}_k^T Q_L^T \widehat{F}_k + \widehat{F}_k^T Q_L \widehat{V}_k - \widehat{F}_k^T \widehat{F}_k + H_k\| = O(c_3(m, n, p)\varepsilon).$$

Therefore,

$$\widehat{B}_k^T (I_k - \widehat{U}_k^T \widehat{U}_k)\widehat{B}_k = (I_k - \widehat{V}_k^T \widehat{V}_k) - P B_k^T (I_{k+1} - U_{k+1}^T U_{k+1}) B_k P + O(\eta).$$

Notice that, in the JBDPRO algorithm, we have $\xi(\widehat{V}_k) = \|I_k - \widehat{V}_k^T \widehat{V}_k\| = O(\eta)$ and $\xi(U_{k+1}) = \|I_{k+1} - U_{k+1}^T U_{k+1}\| = O(\eta)$. We finally obtain

$$\xi(\widehat{U}_k) = \|I_k - \widehat{U}_k^T \widehat{U}_k\| \le \|\widehat{B}_k^{-1}\|^2 [\|B_k\|^2 O(\eta) + O(\eta)] = O(\|\widehat{B}_k^{-1}\|^2 \eta),$$

which is the desired result. □

Since the orthogonality level of $\hat{v}_i$ is $O(\eta)$, which is below $\sqrt{\delta/(2k+1)}$, by Theorem 3.4, the relation (3.20) holds as long as $\kappa(\widehat{U}_k)$ is below $\sqrt{\delta/(2k+1)}$, i.e., the following condition should be satisfied:

$$\|\widehat{B}_k^{-1}\|^2 \varepsilon^{3/4} \lesssim \sqrt{\delta/(2k+1)},$$

which leads to

$$\|\widehat{B}_k^{-1}\|^3 \lesssim \frac{c_4(m, n, p)}{(2k+1)\sqrt{\varepsilon}}. \tag{4.8}$$

Therefore, for the JBDPRO algorithm, if we use some of the singular values of $\widehat{B}_k$ to approximate the desired generalized singular values of $\{A, L\}$, the ghosts can be prevented from appearing as long as the growth of $\|\widehat{B}_k^{-1}\|$ can be controlled by (4.8).

5 Numerical experiments

In this section, we provide several numerical examples to illustrate our theory about the properties of the JBD process with the semiorthogonalization strategy and the JBDPRO algorithm. The matrices are constructed by ourselves or chosen from the University of Florida Sparse Matrix Collection [3]. For the first pair, the matrices A and L, which are denoted by A_c and L_s, respectively, are constructed by ourselves. Let $n = 800$ and $C = diag(c)$, where $c = (\frac{3n}{2}, \frac{3n}{2} - 1, \ldots, \frac{n}{2} + 1)/2n$. Then, let $s = ((1 - c_1^2)^{1/2}, \ldots, (1 - c_n^2)^{1/2})$ and $S = diag(s)$. Let D be the matrix generated by the MATLAB built-in function `D=gallery('orthog',n,2)`, which means that D is a symmetric orthogonal matrix. Finally, let $A = CD$ and $L = SD$. For the second pair, A and L are the square matrices dw2048 and rdb2048 from electromagnetics problems and computational fluid dynamics problems, respectively. For the third pair, A is the square matrix ex31 from computational fluid dynamics problems, $L_m = diag(l)$, where $l = (3m, 3m - 1, \ldots, 2m + 1)/4000$ and m is the row

number of A. For the fourth pair, A is the square matrix rdb5000 from computational fluid dynamics problems and $L = L_1$, which is the discrete approximation of the first-order derivative operator. The properties of our test matrices are described in Table 1, where $cond(\cdot)$ means the condition number of a matrix.

$$L_1 = \begin{pmatrix} 1 & -1 & & \\ & 1 & -1 & \\ & & \ddots & \ddots \\ & & & 1 \quad -1 \end{pmatrix} \in \mathbb{R}^{(n-1)\times n}, \tag{5.1}$$

The numerical experiments are performed on an Intel (R) Core (TM) i7-7700 CPU 3.60GHz with the main memory 8GB using the Matlab R2017b with the machine precision $\varepsilon = 2.22 \times 10^{-16}$ under the Windows 10 operating 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, where m is the row number of A. We mention that our results are based on the assumption that the inner least squares problem (2.1) is solved accurately at each step. Therefore, for the JBD process in the numerical experiments, the QR factorization of $\begin{pmatrix} A \\ L \end{pmatrix}$ is computed, and $QQ^T\tilde{u}_i$ is computed explicitly using Q at each step.

In the JBD process, in order to ensure that $\widetilde{V}_k$ does not deviate far from the column space of Q, the position of the matrices in the matrix pair $\{A, L\}$ may need to be adjusted; see (2.14) and Remark 2.1. Especially, in the four test examples, we implement the JBD process of $\{L_m$,ex31$\}$ instead of $\{$ex31,$L_m\}$.

Figure 1 depicts $\|H_k\| = \|I_k - B_k^T B_k - P\widehat{B}_k^T \widehat{B}_k P\|$ and its upper bound in (3.13) as the iteration number k increases from 1 to 200. Notice (3.18). We use 100ε as the upper bound of $\|H_k\|$. From the four examples, we find that as the matrix orders become bigger, $\|H_k\|$ grows very slightly as the iteration number k increases, due to the fact that $\|H_k\|$ is dependent on the orders of matrices A and L.

Figures 2 and 3 depict the orthogonality levels of u_i, $\tilde{v}_i$, and $\hat{u}_i$ computed by the JBDPRO algorithm. We use the matrix pairs $\{L_m$,ex31$\}$ and $\{$rdb5000,$L_1\}$ to illustrate the results; the results on $\{A_c, L_s\}$ and $\{$rdb2048,dw2048$\}$ are similar and we omit them. The η-criterion is used and $\eta = \varepsilon^{3/4} \approx 10^{-12}$. From the figures we find that in the first few iteration steps, the orthogonality of u_i and $\tilde{v}_i$ lose gradually. Then, the partial reorthogonalization is applied to u_i and $\tilde{v}_i$, making the orthogonality is suddenly recovered, and then the reorthogonalization is not used in a few later steps until the orthogonality levels exceed η again. The algorithm continues in this way

Table 1 Properties of the test matrices

A	$m \times n$	$cond(A)$	L	$p \times n$	$cond(L)$
A_c	800×800	2.99	L_s	800×800	1.46
rdb2048	2048×2048	2026.80	dw2048	2048×2048	5301.50
ex31	3909×3909	1.01×10^6	L_m	3909×3909	1.50
rdb5000	5000×5000	4304.90	L_1	4999×5000	3183.1

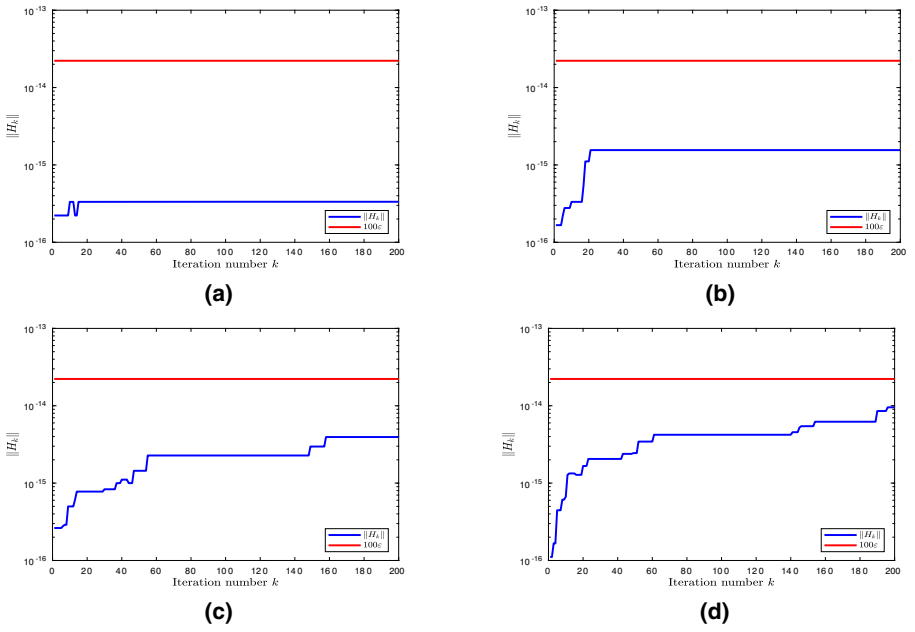

Fig. 1 $\|H_k\|$ and its upper bound: **a** $\{A_c, L_s\}$; **b** {rdb2048,dw2048}; **c** $\{L_m$,ex31$\}$; **d** {rdb5000,L_1}

and the orthogonality levels of u_i and $\tilde{v}_i$ fluctuate around η as the iteration number k continues increasing. We also depict the orthogonality levels of v_i, and we can find that the orthogonality levels of u_i and $\tilde{v}_i$ are almost equal. From Fig. 3, we find that the orthogonality level of $\hat{v}_i$ is mainly affected by the growth of $\|\widehat{B}_k^{-1}\|$. If $\|\widehat{B}_k^{-1}\|$ does not become too large, then the orthogonality of $\hat{u}_i$ will be at a desired level although we do not reorthogonalize any $\hat{v}_i$ in the JBDPRO algorithm.

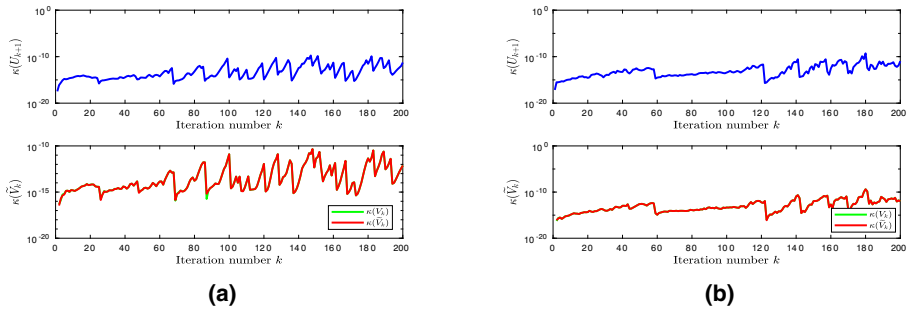

Fig. 2 Orthogonality levels of u_i, $\tilde{v}_i$, and v_i: **a** $\{L_m$,ex31$\}$; **b** {rdb5000,L_1}

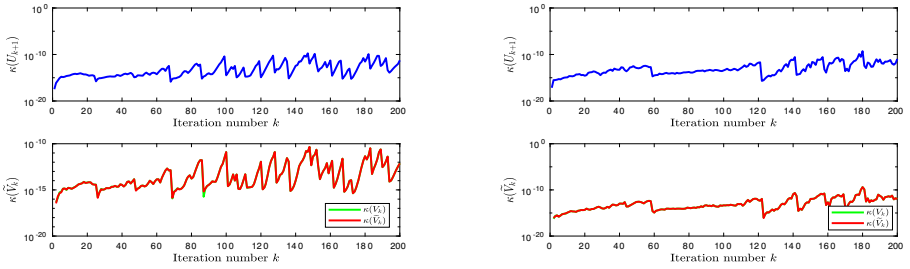

Fig. 3 Orthogonality levels of $\hat{v}_i$: **a** $\{L_m$,ex31$\}$; **b** $\{$rdb5000,$L_1\}$

Now, we compare the JBDPRO algorithm with the JBD with full reorthogonalization (JBDFRO). The JBDFRO algorithm uses the full reorthogonalization strategy for u_i, $\tilde{v}_i$, and $\hat{u}_i$ at each step, and the computed U_{k+1}, $\widetilde{V}_k$, and $\widetilde{U}_k$ are orthogonalized to machine precision ε. Figures 4 and 5 depict the curves of $\|E_k\|$ and $\|\widetilde{E}_k\|$ computed by JBDPRO and JBDFRO, respectively. From these figures, we can observe that both $\|E_k\|$ and $\|\widehat{E}_k\|$ computed by JBDPRO and JBDFRO are almost the same. For each of the four examples, the quantity $\|E_k\|$ does not deviate far from ε and

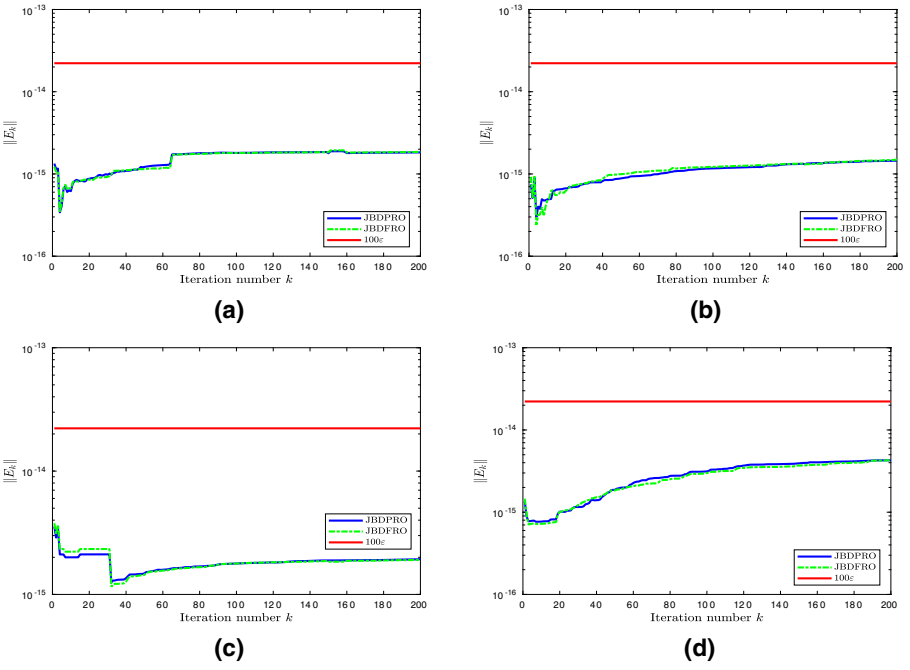

Fig. 4 Comparison of $\|E_k\|$ computed by JBDPRO and JBDFRO: **a** $\{A_c, L_s\}$; **b** $\{$rdb2048,dw2048$\}$; **c** $\{L_m$,ex31$\}$; **d** $\{$rdb5000,$L_1\}$

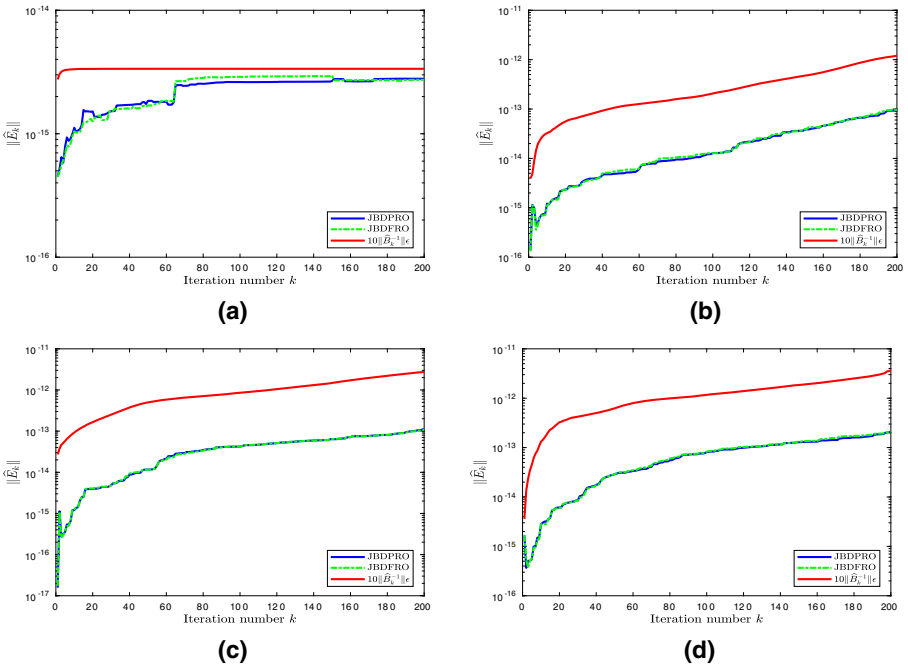

Fig. 5 Comparison of $\|\widehat{E}_k\|$ computed by JBDPRO and JBDFRO: **a** $\{A_c, L_s\}$; **b** {rdb2048,dw2048}; **c** $\{L_m$,ex31$\}$; **d** $\{$rdb5000,$L_1\}$

100ε is an upper bound, while $\|\widehat{E}_k\|$ grows slightly and the growth speed is mainly affected by the size of $\|\widehat{B}_k^{-1}\|$.

We show the convergence of the singular values of B_k or $\widehat{B}_k$ computed by the JBD process with and without the semiorthogonalization strategy, respectively. The matrix pair $\{A, L\}$ is constructed as follows. Let $m = n = p = 800$. First, construct a vector c such that $c(1) = 0.90$, $c(2) = c(3) = 0.86$, $c(4) = 0.82$, $c(5) = 0.78$, $c(796) = 0.22$, $c(797) = 0.20$, $c(798) = c(799) = 0.15$, $c(800) = 0.10$ and `c(6:795)=linspace(0.80,0.30,790)` generated by the MATLAB built-in function `linspace()`. Then, let $s = ((1 - c_1^2)^{1/2}, \ldots, (1 - c_n^2)^{1/2})$ and take $C = diag(c)$, $S = diag(s)$ and `D = gallery('orthog',n,2)`, which means that D is a symmetric orthogonal matrix. Finally, let $A = CD$ and $L = SD$. By the construction, we know that the i-th generalized singular value of $\{A, L\}$ is $\{c_i, s_i\}$, and the multiplicities of the generated singular values $\{0.86, \sqrt{1 - 0.86^2}\}$ and $\{0.15, \sqrt{1 - 0.15^2}\}$ are 2.

Figure 6 depicts the convergence of the first five largest and smallest Ritz values, which are the singular values of B_k computed by the JBD and JBDPRO algorithms, respectively. The right horizontal line indicates the values of c_i for $i = 1, \ldots, 800$. In the left part, which shows the convergence behavior without reorthogonalization, we see the phenomenon that some of the converged Ritz values suddenly "jump"

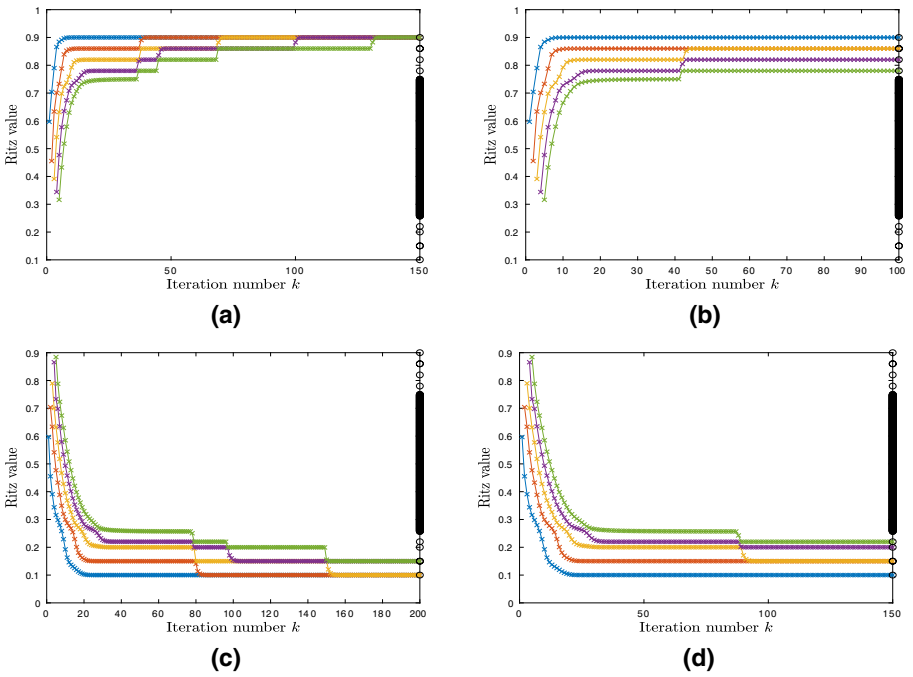

Fig. 6 Convergence of Ritz values from the SVD of B_k: **a** the first five largest Ritz values, computed by JBD; **b** the first five largest Ritz values, computed by JBDPRO; **c** the first five smallest Ritz values, computed by JBD; **d** the first five smallest Ritz values, computed by JBDPRO

and become "ghosts" and then converge to the next larger or smaller singular values after a few iterations, which results in many unwanted spurious copies of generalized singular values and makes it difficult to determine whether these spurious copies are genuine multiple generalized singular values. In the right part, where B_k is computed by the JBDPRO algorithm, the convergence behavior is much simpler and it is similar to the ideal case in exact arithmetic. It can be found from subfigures (b) and (d) that a simple generalized singular value can be approximated by Ritz values with no ghost appearing, while a multiple generalized singular value can be approximated one by one by the Ritz values.

Figure 7 depicts the convergence of the first five largest and smallest Ritz values from the SVD of $\widehat{B}_k$, where the right horizontal line indicates the value of s_i for $i = 1, \ldots, 800$. The convergence behavior of the Ritz values from the SVD of $\widehat{B}_k$ is very similar to that from the SVD of B_k. From subfigures (a) and (c), which show the convergence of Ritz values without reorthogonalization, we find the "ghosts" phenomenon that some converged Ritz values suddenly "jump" and then converge to the next larger or smaller singular values after a few iterations. In subfigures (b) and (d), where $\widehat{B}_k$ is computed by the JBDPRO algorithm, there are no spurious copies, and the multiplicities of the generalized singular values can be determined correctly from the convergence of Ritz values.

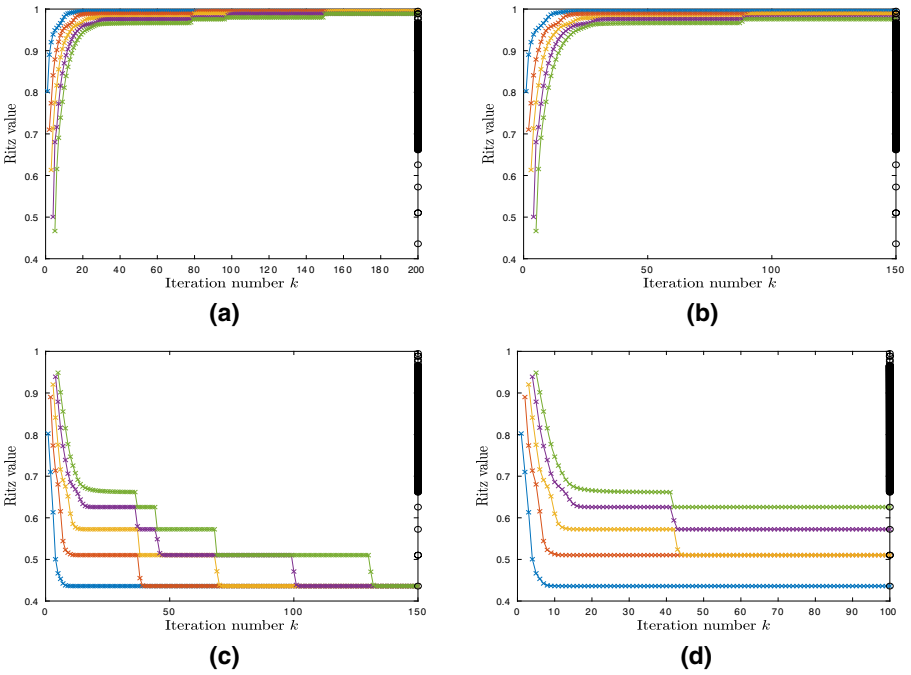

Fig. 7 Convergence of Ritz values from the SVD of $\widehat{B}_k$: **a** the first five largest Ritz values, computed by JBD; **b** the first five largest Ritz values, computed by JBDPRO; **c** the first five smallest Ritz values,computed by JBD; **d** the first five smallest Ritz values, computed by JBDPRO

Finally, we compare the efficiency of the JBDPRO and JBDFRO. Table 2 shows the running time of 200-step JBD, JBDPRO, and JBDFRO for the four test examples. We also compute the ratio of the running times of JBDPRO and JBDFRO. For each case, we run the algorithms 10 times and take the average over all 10 running times. From the table, we find that the running time of JBDPRO is only about 70–80% of that of JBDFRO. Therefore, the JBDPRO is more efficient than JBDFRO, but can prevent "ghosts" from appearing.

Table 2 Running time comparison (measured in seconds)

A	L	JBD	JBDPRO	JBDFRO	Ratio (%)
A_c	L_s	0.2528	0.2639	0.4801	54.98
rdb2048	dw2048	2.0048	2.2476	2.7790	80.88
L_m	ex31	6.8089	7.0218	9.4157	74.58
rdb5000	L_1	10.4968	10.7883	14.2574	75.67

6 Conclusion

We have proposed a semiorthogonalization strategy for the JBD process to maintain some level of orthogonality of the Lanczos vectors. Our rounding error analysis establishes connections between the JBD process with the semiorthonalization strategy and the Lanczos bidiagonalization process. We have proved that if the Lanczos vectors are kept semiorthogonal, then the computed $\widehat{B}_k$ is the Ritz-Galerkin projection of Q_L on the subspaces $span(\widehat{U}_k)$ and $span(\widehat{V}_k)$ within error $\delta = O(c_4(m,n,p)\|\widehat{B}_k^{-1}\|\varepsilon)$. Therefore, the convergence of Ritz values computed from $\widehat{B}_k$ will not be affected by rounding errors and the final accuracy of computed quantities is high enough as long as $\|\widehat{B}_k^{-1}\|$ does not become too large.

Based on the semiorthogonalization strategy, we have developed the JBDPRO algorithm. The JBDPRO algorithm can keep the orthogonality of Lanczos vectors and saves much unnecessary reorthogonalization work compared with the JBDFRO algorithm. Several numerical examples have been used to confirm our theory and the algorithmic behavior in finite precision arithmetic.

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Appendix 1: Proofs of Lemma 3.1 and Lemma 3.2

Proof of Lemma 3.1 We prove (3.11) by mathematical induction. For $i = 1$, from (3.9) and (3.10), we have

$$\begin{aligned}\hat{\alpha}_1 Q_L^T \hat{u}_1 &= Q_L^T Q_L \hat{v}_1 - Q_L^T \hat{f}_1 \\ &= (I_n - Q_A^T Q_A)\hat{v}_1 - Q_L^T \hat{f}_1 \\ &= \hat{v}_1 - Q_A^T(\alpha_1 u_1 + \beta_2 u_2 + f_1) - Q_L^T \hat{f}_1 \\ &= \hat{v}_1 - \alpha_1(\alpha_1 v_1 + g_1) - \beta_2(\alpha_2 v_2 + \beta_2 v_1 + g_2) - Q_A^T f_1 - Q_L^T \hat{f}_1 \\ &= (1 - \alpha_1^2 - \beta_2^2)\hat{v}_1 + \alpha_2\beta_2\hat{v}_2 + O(\bar{q}(m,n,p)\varepsilon).\end{aligned}$$

Next, suppose (3.11) is true for the indices up to i. For $i+1$, we have

$$\hat{\alpha}_{i+1} Q_L^T \hat{u}_{i+1} = Q_L^T Q_L \hat{v}_{i+1} - \hat{\beta}_i Q_L^T \hat{u}_i - \sum_{j=1}^{i-1} \hat{\xi}_{ji+1} Q_L^T \hat{u}_j - Q_L^T \hat{f}_{i+1}.$$

Since $(\hat{\beta}_i Q_L^T \hat{u}_i - \sum_{j=1}^{i-1} \hat{\xi}_{ji+1} Q_L^T \hat{u}_j) \in span\{\hat{v}_1, \ldots, \hat{v}_{i+1}\} + O(\bar{q}(m,n,p)\varepsilon)$, we only need to prove $Q_L^T Q_L \hat{v}_{i+1} \in span\{\hat{v}_1, \ldots, \hat{v}_{i+2}\} + O(\bar{q}(m,n,p)\varepsilon)$. Notice that

$$\begin{aligned}Q_L^T Q_L \hat{v}_{i+1} &= (I_n - Q_A^T Q_A)\hat{v}_{i+1} \\ &= \hat{v}_{i+1} + (-1)^{i+1} Q_A^T(\alpha_{i+1} u_{i+1} + \beta_{i+1} u_{i+2} + \sum_{j=1}^{i} \xi_{ji+1} u_j + f_{i+1})\end{aligned}$$

$$= \hat{v}_{i+1} + (-1)^{i+1}(\alpha_{i+1} Q_A^T u_{i+1} + \beta_{i+1} Q_A^T u_{i+2} + \sum_{j=1}^{i} \xi_{ji+1} Q_A^T u_j)$$
$$+(-1)^{i+1} Q_A^T f_{i+1}.$$

From (3.9), we have

$$(\alpha_{i+1} Q_A^T u_{i+1} + \beta_{i+1} Q_A^T u_{i+2} + \sum_{j=1}^{i} \xi_{ji+1} Q_A^T u_j) \in span\{\hat{v}_1, \ldots, \hat{v}_{i+2}\} + O(\bar{q}(m, n, p)\varepsilon),$$

which completes the proof of the induction step.

By the mathematical induction principle, (3.11) holds for all $i = 1, 2, \ldots, k$. □

Proof of Lemma 3.2 By (3.8) and (3.9), the process of computing U_{k+1} and V_k can be treated as the Lanczos bidiagonalization of Q_A with the semiorthogonalization strategy. Since the k-step Lanczos bidiagonalization process is equivalent to the $(2k + 1)$-step symmetric Lanczos process [2, §7.6.1], the bounds for C_k and D_k can be deduced from the property of the symmetric Lanczos process with the semiorthogonalization strategy; see [26, Lemma 4] and its proof.

Now, we give the bound of $\widehat{C}_k$. At the $(i - 1)$-th step, from (3.10), we can write the reorthogonalization step of $\hat{u}_i$ as

$$\hat{\alpha}_i' \hat{u}_i' = Q_L \hat{v}_i - \hat{\beta}_{i-1} \hat{u}_{i-1} - \hat{f}_i', \tag{A.1}$$
$$\hat{\alpha}_i \hat{u}_i = \hat{\alpha}_i' \hat{u}_i' - \textstyle\sum_{j=1}^{i-2} \hat{\xi}_{ji} \hat{u}_j - \hat{f}_i'', \tag{A.2}$$

where $\|\hat{f}_i'\|, \|\hat{f}_i''\| = O(q_3(p, n)\varepsilon)$. Thus, for $l = 1, \ldots, i - 2$, we have

$$\hat{\alpha}_i' \hat{u}_l^T \hat{u}_i' = \hat{u}_l^T Q_L \hat{v}_i - \hat{\beta}_{i-1} \hat{u}_l^T \hat{u}_{i-1} - \hat{u}_l^T \hat{f}_i'.$$

From (3.11) and its proof, we know that

$$Q_L^T \hat{u}_l = \sum_{j=1}^{l+1} \lambda_j \hat{v}_j + O(\bar{q}(m, n, p)\varepsilon)$$

with modest constants λ_j for $j = 1, \ldots, l + 1$. Notice that $\left|\hat{u}_l^T \hat{u}_{i-1}, \hat{v}_j^T \hat{v}_i\right| \leq \sqrt{\varepsilon/(2k + 1)}$ for $l = 1, \ldots, i - 2$ and $j = 1, \ldots, l + 1$. We obtain

$$\hat{\alpha}_i' \hat{u}_l^T \hat{u}_i' = \sum_{j=1}^{l+1} \lambda_j \hat{v}_j^T \hat{v}_i - \hat{\beta}_{i-1} \hat{u}_l^T \hat{u}_{i-1} + O(\bar{q}(m, n, p)\varepsilon) = O(\sqrt{\varepsilon}).$$

Then, we prove $M = \max_{1 \leq j \leq i-1} |\hat{\xi}_{ji}| = O(\sqrt{\varepsilon})$. Premultiplying (A.1) by $\hat{u}_l^T$ and making some arrangement, we obtain

$$\hat{\xi}_{li} = \hat{\alpha}_i' \hat{u}_l^T \hat{u}_i' - \hat{\alpha}_i \hat{u}_l^T \hat{u}_i - \sum_{j=1, j \neq l}^{i-2} \hat{\xi}_{ji} \hat{u}_l^T \hat{u}_j - \hat{u}_l^T \hat{f}_i''.$$

Notice that $\hat{u}_l^T \hat{u}_i = O(\sqrt{\varepsilon})$ and we have proved $\hat{\alpha}_i' \hat{u}_l^T \hat{u}_i' = O(\sqrt{\varepsilon})$ for $l = 1, \ldots, i-2$. We obtain

$$|\hat{\xi}_{li}| \leq O(\sqrt{\varepsilon}) + O(\sqrt{\varepsilon}) + iM\sqrt{\varepsilon} + O(\bar{q}(m, n, p)\varepsilon).$$

The above right-hand side does not depend on l anymore, and we finally obtain by taking the maximum on the the left-hand side:

$$(1 - i\sqrt{\varepsilon})M \leq O(\sqrt{\varepsilon}) + O(\bar{q}(m, n, p)\varepsilon).$$

Therefore, we have $M = O(\sqrt{\varepsilon})$. □

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