TWO HARMONIC JACOBI–DAVIDSON METHODS FOR COMPUTING A PARTIAL GENERALIZED SINGULAR VALUE DECOMPOSITION OF A LARGE MATRIX PAIR*

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Abstract. Two harmonic extraction based Jacobi–Davidson (JD) type algorithms are proposed to compute a partial generalized singular value decomposition (GSVD) of a large regular matrix pair. They are called cross product-free (CPF) and inverse-free (IF) harmonic JDGSVD algorithms, abbreviated as CPF-HJDGSVD and IF-HJDGSVD, respectively. Compared with the standard extraction based JDGSVD algorithm, the harmonic extraction based algorithms converge more regularly and suit better for computing GSVD components corresponding to interior generalized singular values. Thick-restart CPF-HJDGSVD and IF-HJDGSVD algorithms with some deflation and purgation techniques are developed to compute more than one GSVD components. Numerical experiments confirm the superiority of CPF-HJDGSVD and IF-HJDGSVD to the standard extraction based JDGSVD algorithm.

Key words. Generalized singular value decomposition, generalized singular value, generalized singular vector, standard extraction, harmonic extraction, Jacobi–Davidson type method

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1. Introduction. For a pair of large and possibly sparse matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{p \times n}$, the matrix pair (A, B) is called regular if $\mathcal{N}(A) \cap \mathcal{N}(B) = \{\mathbf{0}\}$, i.e., rank $\left(\begin{bmatrix} A \\ B \end{bmatrix}\right) = n$, where $\mathcal{N}(A)$ and $\mathcal{N}(B)$ denote the null spaces of A and B, respectively. The generalized singular value decomposition (GSVD) of (A, B) was introduced by Van Loan [34] and developed by Paige and Saunders [28]. Since then, GSVD has become a standard matrix decomposition and has been widely used [2, 3, 4, 9, 10, 25]. Let $q_1 = \dim(\mathcal{N}(A))$, $q_2 = \dim(\mathcal{N}(B))$ and $l_1 = \dim(\mathcal{N}(A^T))$, $l_2 = \dim(\mathcal{N}(B^T))$, where the superscript T denotes the transpose. Then the GSVD of (A, B) is

(1.1)
$$\begin{cases} U^T A X = \Sigma_A = \text{diag}\{C, \mathbf{0}_{l_1, q_1}, I_{q_2}\}, \\ V^T B X = \Sigma_B = \text{diag}\{S, I_{q_1}, \mathbf{0}_{l_2, q_2}\}, \end{cases}$$

where $X = [X_q, X_{q_1}, X_{q_2}]$ is nonsingular, $U = [U_q, U_{l_1}, U_{q_2}]$ and $V = [V_q, V_{q_1}, V_{l_2}]$ are orthogonal, and the diagonal matrices $C = \text{diag}\{\alpha_1, \ldots, \alpha_q\}$ and $S = \text{diag}\{\beta_1, \ldots, \beta_q\}$ satisfy

$$0 < \alpha_i, \beta_i < 1$$
 and $\alpha_i^2 + \beta_i^2 = 1, \quad i = 1, \dots, q$

with $q = n - q_1 - q_2$. Here, $\mathbf{0}_{l_i,q_i}$ and $I_{q_i}, i = 1, 2$, are the $l_i \times q_i$ zero matrices and identity matrices of order q_i , respectively; see [28]. The GSVD part in (1.1) that corresponds to α_i and β_i can be written as

(1.2)
$$\begin{cases} Ax_i = \alpha_i u_i, \\ Bx_i = \beta_i v_i, \\ \beta_i A^T u_i = \alpha_i B^T v_i, \end{cases} i = 1, \dots, q,$$

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where x_i is the *i*th column of X_q and the unit-length vectors u_i and v_i are the *i*th columns of U_q and V_q , respectively. The quintuples $(\alpha_i, \beta_i, u_i, v_i, x_i)$, $i = 1, \ldots, q$ are called nontrivial GSVD components of (A, B). Particularly, the numbers $\sigma_i = \frac{\alpha_i}{\beta_i}$ or the pairs (α_i, β_i) are called the nontrivial generalized singular values, and u_i, v_i and x_i are the corresponding left and right generalized singular vectors, respectively, $i = 1, \ldots, q$.

For a given target $\tau > 0$, we assume that all the nontrivial generalized singular values of (A, B) are labeled by their distances from τ :

$$(1.3) |\sigma_1 - \tau| \le \dots \le |\sigma_\ell - \tau| < |\sigma_{\ell+1} - \tau| \le \dots \le |\sigma_q - \tau|.$$

We are interested in computing the GSVD components $(\alpha_i, \beta_i, u_i, v_i, x_i)$ corresponding to the ℓ nontrivial generalized singular values σ_i of (A, B) closest to τ . If τ is inside the nontrivial generalized singular spectrum of (A, B), then $(\alpha_i, \beta_i, u_i, v_i, x_i)$, $i = 1, \ldots, \ell$ are called interior GSVD components of (A, B); otherwise, they are called the extreme, i.e., largest or smallest, ones. A large number of GSVD components, some of which are interior ones [5, 6, 7], are required in a variety of applications. Throughout this paper, we assume that τ is not equal to any generalized singular value of (A, B).

Zha [37] proposes a joint bidiagonalization (JBD) method to compute extreme GSVD components of the large matrix pair (A, B). The method is based on a JBD process that successively reduces (A, B) to a sequence of upper bidiagonal pairs, from which approximate GSVD components are computed. Kilmer, Hansen and Espanol [26] have adapted the JBD process to the linear discrete ill-posed problem with general-form regularization and developed a JBD process that reduces (A, B) to lower-upper bidiagonal forms. Jia and Yang [24] have developed a new JBD process based iterative algorithm for the ill-posed problem and considered the convergence of extreme generalized singular values. In the GSVD computation and the solution of discrete ill-posed problem, one needs to solve an $(m+p) \times n$ least squares problem with the coefficient matrix $[A^T, B^T]^T$ at each step of the JBD process. Jia and Li [22] have recently considered the JBD process in finite precision and proposed a partial reorthogonalization strategy to maintain numerical semi-orthogonality among the generated basis vectors so as to avoid ghost approximate GSVD components, where the semi-orthogonality means that two unit-length vectors are numerically orthogonal to the level of $\epsilon_{\rm mach}^{1/2}$ with $\epsilon_{\rm mach}$ being the machine precision.

Hochstenbach [12] presents a Jacobi-Davidson (JD) GSVD (JDGSVD) method to compute a number of interior GSVD components of (A, B) with B of full column rank, where, at each step, an (m+n)-dimensional linear system, i.e., the correction equation, needs to be solved iteratively with low or modest accuracy; see [14, 15, 20, 21]. The lower n-dimensional and upper m-dimensional parts of the approximate solution are used to expand the right and one of the left searching subspaces, respectively. The JDGSVD method formulates the GSVD of (A, B) as the equivalent generalized eigendecomposition of the augmented matrix pair $(\begin{bmatrix} A \end{bmatrix}, \begin{bmatrix} I \end{bmatrix}, \begin{bmatrix} I \end{bmatrix}$ for B of full column rank, computes the relevant eigenpairs, and recovers the approximate GSVD components from the converged eigenpairs. The authors [16] have shown that the error of the computed eigenvector is bounded by the size of the perturbations times a multiple $\kappa(B^T B) = \kappa^2(B)$, where $\kappa(B) = \sigma_{\max}(B)/\sigma_{\min}(B)$ denotes the 2-norm condition number of B with $\sigma_{\max}(B)$ and $\sigma_{\min}(B)$ being the largest and smallest singular values of B, respectively. Consequently, with an ill-conditioned B, the computed GSVD components may have very poor accuracy, which has been numerically confirmed [16]. The results in [16] show that if B is ill conditioned but A has full column rank and is well conditioned then the JDGSVD method can be applied to the matrix pair ($\begin{bmatrix} B \end{bmatrix}$, $\begin{bmatrix} I \\ A^T A \end{bmatrix}$) and computes the corresponding approximate GSVD components with high accuracy. Note that the two formulations require that B and A be rectangular or square, respectively. We should also realize that a reliable estimation of the condition numbers of A and B may be costly, so that it may be difficult to choose a proper formulation in applications.

Zwaan and Hochstenbach [39] present a generalized Davidson (GDGSVD) method and a multidirectional (MDGSVD) method to compute an extreme partial GSVD of (A,B). These two methods involve no cross product matrices A^TA and B^TB or matrix-matrix products, and they apply the standard extraction approach, i.e., the Rayleigh-Ritz method [31] to (A, B) directly and compute approximate GSVD components with respect to the given left and right searching subspaces, where the two left subspaces are formed by premultiplying the right one with A and B, respectively. At iteration k of the GDGSVD method, the right searching subspace is spanned by the k residuals of the generalized Davidson method [1, Sec. 11.2.4 and Sec. 11.3.6] applied to the generalized eigenvalue problem of (A^TA, B^TB) ; in the MDGSVD method, an inferior search direction is discarded by a truncation technique, so that the searching subspaces are improved. Zwaan [38] exploits the Kronecker canonical form of a regular matrix pair [32] and shows that the GSVD problem of (A, B) can be formulated as a certain $(2m+p+n)\times(2m+p+n)$ generalized eigenvalue problem without involving any cross product or any other matrix-matrix product. Such formulation currently is mainly of theoretical value since the nontrivial eigenvalues and eigenvectors of the structured generalized eigenvalue problem are always complex: the generalized eigenvalues are the conjugate quaternions $(\sqrt{\sigma_j}, -\sqrt{\sigma_j}, i\sqrt{\sigma_j}, -i\sqrt{\sigma_j})$ with i the imaginary unit, and the corresponding right generalized eigenvectors are

$$[u_j^T, x_j^T/\beta_j, \sqrt{\sigma_j} u_j^T, \sqrt{\sigma_j} v_j^T]^T, \qquad [-u_j^T, -x_j^T/\beta_j, \sqrt{\sigma_j} u_j^T, \sqrt{\sigma_j} v_j^T]^T,$$

$$[-iu_j^T, ix_j^T/\beta_j, \sqrt{\sigma_j} u_j^T, -\sqrt{\sigma_j} v_j^T]^T, \qquad [iu_j^T, ix_j^T/\beta_j, -\sqrt{\sigma_j} u_j^T, -\sqrt{\sigma_j} v_j^T]^T.$$

Clearly, the size of the generalized eigenvalue problem is much bigger than that of the GSVD of (A,B). The conditioning of eigenvalues and eigenvectors of this problem is also unclear. In the meantime, no structure-preserving algorithm has been found for such kind of complicated structured generalized eigenvalue problem. Definitely, it will be extremely difficult and highly challenging to seek for a numerically stable structure-preserving algorithm for this problem.

The authors [15] have recently proposed a Cross Product-Free JDGSVD method, referred to as the CPF-JDGSVD method, to compute several GSVD components of (A, B) corresponding to the generalized singular values closest to τ . The CPF-JDGSVD method is cross products A^TA and B^TB free when constructing and expanding right and left searching subspaces; it premultiplies the right searching subspace by A and B to construct two left ones separately, and forms the orthonormal bases of those by computing two thin QR factorizations, as done in [39]. The resulting projected problem is the GSVD of a small matrix pair without involving any cross product or matrix-matrix product. Mathematically, the method implicitly deals with the equivalent generalized eigenvalue problem of (A^TA, B^TB) without forming A^TA or B^TB explicitly. At the subspace expansion stage, an n-by-n correction equation is approximately solved iteratively with low or modest accuracy, and the approximate solution is used to expand the searching subspaces. Therefore, the subspace expansion is fundamentally different from that used in [39], where the dimension n of the correction equations is no more than half of the dimension m + n of those in [12].

Just like the standard Rayleigh-Ritz method for the matrix eigenvalue problem and the singular value decomposition (SVD) problem, the CPF-JDGSVD method suits better for the computation of some extreme GSVD components, but it may encounter some serious difficulties for the computation of interior GSVD components. Remarkably, adapted from the standard extraction approach for the eigenvalue problem and SVD problem to the GSVD computation, an intrinsic shortcoming of a standard extraction based method is that it may be hard to pick up good approximate generalized singular values correctly even if the searching subspaces are sufficiently good. This potential disadvantage may make the resulting algorithm expand the subspaces along wrong directions and converge irregularly, as has been numerically observed in [15]. To this end, inspired by the harmonic extraction based methods that suit better for computing interior eigenpairs and SVD components [11, 13, 14, 17, 23, 21, 27], we will propose two harmonic extraction based JDGSVD methods that are particularly suitable for the computation of interior GSVD components. One method is cross products $A^T A$ and $B^T B$ free, and the other is inversions $(A^T A)^{-1}$ and $(B^T B)^{-1}$ free. As will be seen, the derivations of the two harmonic extraction methods are nontrivial. and they are subtle adaptations of the harmonic extraction for matrix eigenvalue and SVD problems. In the sequel, we will abbreviate Cross Product-Free and Inverse-Free Harmonic JDGSVD methods as CPF-HJDGSVD and IF-HJDGSVD, respectively.

We first focus on the case $\ell=1$ and propose our harmonic extraction based JDGSVD type methods. Then by introducing the deflation technique in [15] into the methods, we present the methods to compute more than one, i.e., $\ell>1$, GSVD components. To be practical, combining the thick-restart technique in [30] and some purgation approach, we develop thick-restart CPF-HJDGSVD and IF-HJDGSVD algorithms to compute the ℓ GSVD components associated with the generalized singular values of (A,B) closest to τ .

The rest of this paper is organized as follows. In Section 2, we briefly review the CPF-JDGSVD method proposed in [15]. In Section 3, we propose the CPF-HJDGSVD and IF-HJDGSVD methods. In Section 4, we develop thick-restart CPF-HJDGSVD and IF-HJDGSVD with deflation and purgation to compute ℓ GSVD components of (A,B). In Section 5, we report numerical experiments to illustrate the performance of CPF-HJDGSVD and IF-HJDGSVD, make a comparison of them and CPF-JDGSVD, and show the superiority of the former two to the latter one. Finally, we conclude the paper in Section 6.

Throughout this paper, we denote by $\mathcal{R}(\cdot)$ the column space of a matrix, and by $\|\cdot\|$ and $\|\cdot\|_1$ the 2- and 1-norms of a matrix or vector, respectively. As in (1.1), we denote by I_i and $\mathbf{0}_{i,j}$ the *i*-by-*i* identity and *i*-by-*j* zero matrices, respectively, with the subscripts i and j dropped whenever they are clear from the context.

2. The standard extraction based JDGSVD method. We review the CPF-JDGSVD method in [15] for computing the GSVD component $(\alpha_*, \beta_*, u_*, v_*, x_*) := (\alpha_1, \beta_1, u_1, v_1, x_1)$ of (A, B). Assume that a k-dimensional right searching subspace $\mathcal{X} \subset \mathbb{R}^n$ is available, from which an approximation to x_* is extracted. Then we construct

(2.1)
$$\mathcal{U} = A\mathcal{X}$$
 and $\mathcal{V} = B\mathcal{X}$

as the two left searching subspaces, from which approximations to u_* and v_* are computed. It is proved in [15] that the distance between u_* and \mathcal{U} (resp. v_* and \mathcal{V}) is as small as that between x_* and \mathcal{X} , provided that α_* (resp. β_*) is not very small. In other words, for the extreme and interior GSVD components, \mathcal{U} and \mathcal{V} constructed by

(2.1) are as good as \mathcal{X} provided that the desired generalized singular values $\sigma_* = \frac{\alpha_*}{\beta_*}$ are neither very small nor very small. It is also proved in [15] that \mathcal{U} or \mathcal{V} is as accurate as \mathcal{X} for very large or small generalized singular values.

Assume that the columns of $\widetilde{X} \in \mathbb{R}^{n \times k}$ form an orthonormal basis of \mathcal{X} , and compute the thin QR factorizations of $A\widetilde{X}$ and $B\widetilde{X}$:

(2.2)
$$A\widetilde{X} = \widetilde{U}R_A$$
 and $B\widetilde{X} = \widetilde{V}R_B$,

where $\widetilde{U} \in \mathbb{R}^{m \times k}$ and $\widetilde{V} \in \mathbb{R}^{p \times k}$ are orthonormal, and $R_A \in \mathbb{R}^{k \times k}$ and $R_B \in \mathbb{R}^{k \times k}$ are upper triangular. Then the columns of \widetilde{U} and \widetilde{V} are orthonormal bases of \mathcal{U} and \mathcal{V} , respectively. With $\mathcal{X}, \mathcal{U}, \mathcal{V}$ and their orthonormal bases available, we can extract an approximation to the desired GSVD component $(\alpha_*, \beta_*, u_*, v_*, x_*)$ of (A, B) with respect to them. The standard extraction approach in [15] seeks for positive pairs $(\widetilde{\alpha}, \widetilde{\beta})$ with $\widetilde{\alpha}^2 + \widetilde{\beta}^2 = 1$, normalized vectors $\widetilde{u} \in \mathcal{U}, \ \widetilde{v} \in \mathcal{V}$, and vectors $\widetilde{x} \in \mathcal{X}$ that satisfy the Galerkin type conditions:

(2.3)
$$\begin{cases} A\tilde{x} - \tilde{\alpha}\tilde{u} \perp \mathcal{U}, \\ B\tilde{x} - \tilde{\beta}\tilde{v} \perp \mathcal{V}, \\ \tilde{\beta}A^T\tilde{u} - \tilde{\alpha}B^T\tilde{v} \perp \mathcal{X}. \end{cases}$$

Among k pairs $(\tilde{\alpha}, \tilde{\beta})$'s, select $\tilde{\theta} = \tilde{\alpha}/\tilde{\beta}$ closest to τ , and take $(\tilde{\alpha}, \tilde{\beta}, \tilde{u}, \tilde{v}, \tilde{x})$ as an approximation to $(\alpha_*, \beta_*, u_*, v_*, x_*)$. We call $(\tilde{\alpha}, \tilde{\beta})$ or $\tilde{\theta} = \frac{\tilde{\alpha}}{\tilde{\beta}}$ a Ritz value and \tilde{u}, \tilde{v} and \tilde{x} the corresponding left and right Ritz vectors, respectively.

It follows from the thin QR factorizations (2.2) of $A\widetilde{X}$ and $B\widetilde{X}$ that $R_A = \widetilde{U}^T A\widetilde{X}$ and $R_B = \widetilde{V}^T A\widetilde{X}$. Write $\widetilde{u} = \widetilde{U}\widetilde{e}$, $\widetilde{v} = \widetilde{V}\widetilde{f}$ and $\widetilde{x} = \widetilde{X}\widetilde{d}$. Then (2.3) becomes

(2.4)
$$R_A \tilde{d} = \tilde{\alpha} \tilde{e}, \qquad R_B \tilde{d} = \tilde{\beta} \tilde{f}, \qquad \tilde{\beta} R_A^T \tilde{e} = \tilde{\alpha} R_B^T \tilde{f},$$

which is precisely the GSVD of the projected matrix pair (R_A, R_B) . Therefore, in the extraction phase, the standard extraction approach computes the GSVD of the k-by-k matrix pair (R_A, R_B) , picks up the GSVD component $(\tilde{\alpha}, \tilde{\beta}, \tilde{e}, \tilde{f}, \tilde{d})$ with $\tilde{\theta} = \frac{\tilde{\alpha}}{\tilde{\beta}}$ being the generalized singular value of (R_A, R_B) closest to the target τ , and use

$$(\tilde{\alpha},\tilde{\beta},\tilde{u},\tilde{v},\tilde{x})=(\tilde{\alpha},\tilde{\beta},\widetilde{U}\tilde{e},\widetilde{V}\tilde{f},\widetilde{X}\tilde{d})$$

as an approximation to $(\alpha_*, \beta_*, u_*, v_*, x_*)$ of (A, B). It is straightforward from (2.3) that $A\tilde{x} = \tilde{\alpha}\tilde{u}$, $B\tilde{x} = \tilde{\beta}\tilde{v}$ and

$$(A^T A - \tilde{\theta}^2 B^T B) \tilde{x} \perp \mathcal{X}.$$

That is, $(\tilde{\theta}^2, \tilde{x})$ is a standard Ritz pair to the eigenpair (σ_*^2, x_*) of the symmetric definite matrix pair (A^TA, B^TB) with respect to the subspace \mathcal{X} . Because of this, we call $(\tilde{\alpha}, \tilde{\beta}, \tilde{u}, \tilde{v}, \tilde{x})$ a standard Ritz approximation in the GSVD context.

Since $A\tilde{x} = \tilde{\alpha}\tilde{u}$ and $B\tilde{x} = \tilde{\beta}\tilde{v}$, the residual of Ritz approximation $(\tilde{\alpha}, \tilde{\beta}, \tilde{u}, \tilde{v}, \tilde{x})$ is

(2.5)
$$r = r(\tilde{\alpha}, \tilde{\beta}, \tilde{u}, \tilde{v}, \tilde{x}) = \tilde{\beta} A^T \tilde{u} - \alpha B^T \tilde{v}.$$

Obviously, $(\tilde{\alpha}, \tilde{\beta}, \tilde{u}, \tilde{v}, \tilde{x})$ is an exact GSVD component of (A, B) if and only if ||r|| = 0. The approximate GSVD component $(\tilde{\alpha}, \tilde{\beta}, \tilde{u}, \tilde{v}, \tilde{x})$ is claimed to have converged if

(2.6)
$$||r|| \le (\tilde{\beta}||A||_1 + \tilde{\alpha}||B||_1) \cdot tol,$$

where tol > 0 is a user prescribed tolerance, and one then stops the iterations.

If $(\tilde{\alpha}, \hat{\beta}, \tilde{u}, \tilde{v}, \tilde{x})$ has not yet converged, the CFP-JDGSVD method expands the right searching subspace \mathcal{X} and constructs the corresponding left subspaces \mathcal{U} and \mathcal{V} by (2.1). Specifically, the CPF-JDGSVD seeks for an expansion vector t in the following way: For the vector

$$\tilde{y} := (A^T A + B^T B)\tilde{x} = \tilde{\alpha} A^T \tilde{u} + \tilde{\beta} B^T \tilde{v}$$

that satisfies $\tilde{y}^T \tilde{x} = 1$, we first solve the correction equation

$$(2.8) (I - \tilde{y}\tilde{x}^T)(A^T A - \rho^2 B^T B)(I - \tilde{x}\tilde{y}^T)t = -r$$

with the fixed $\rho = \tau$ for $t \perp \tilde{y}$ until

(2.9)
$$||r|| \le (\tilde{\beta}||A||_1 + \tilde{\alpha}||B||_1) \cdot fixtol$$

for a user prescribed tolerance fixtol > 0, say, $fixtol = 10^{-4}$, and then solve the modified correction equation with the dynamic $\rho = \tilde{\alpha}/\tilde{\beta}$ for $t \perp \tilde{y}$. Note that $I - \tilde{y}\tilde{x}^T$ is an oblique projector onto the orthogonal complement of the subspace span $\{x\}$.

With the solution t of (2.8), we expand \mathcal{X} to the new (k+1)-dimensional $\mathcal{X}_{\text{new}} = \text{span}\{\widetilde{X},t\}$, whose orthonormal basis matrix is

(2.10)
$$\widetilde{X}_{\text{new}} = [\widetilde{X}, x_{+}] \quad \text{with} \quad x_{+} = \frac{(I - \widetilde{X}\widetilde{X}^{T})t}{\|(I - \widetilde{X}\widetilde{X}^{T})t\|},$$

where x_+ is called an expansion vector. We then compute the orthonormal bases $\widetilde{U}_{\text{new}}$ and $\widetilde{V}_{\text{new}}$ of the expanded left searching subspaces

$$\mathcal{U}_{\text{new}} = A\mathcal{X}_{\text{new}} = \text{span}\{\widetilde{U}, Ax_{+}\}, \qquad \mathcal{V}_{\text{new}} = B\mathcal{X}_{\text{new}} = \text{span}\{\widetilde{V}, Bx_{+}\}$$

by efficiently updating the thin QR factorizations of $A\widetilde{X}_{\text{new}} = \widetilde{U}_{\text{new}} R_{A,\text{new}}$ and $B\widetilde{X}_{\text{new}} = \widetilde{V}_{\text{new}} R_{B,\text{new}}$, respectively, where

$$\widetilde{U}_{\text{new}} = [\widetilde{U}, u_+], \quad R_{A, \text{new}} = \begin{bmatrix} R_A & r_A \\ & \gamma_A \end{bmatrix}, \quad \widetilde{V}_{\text{new}} = [\widetilde{V}, v_+], \quad R_{B, \text{new}} = \begin{bmatrix} R_B & r_B \\ & \gamma_B \end{bmatrix}$$

with

$$r_A = \widetilde{U}^T A x_+, \qquad \gamma_A = \|A x_+ - \widetilde{U} r_A\|, \qquad u_+ = \frac{A x_+ - \widetilde{U} r_A}{\gamma_A},$$

$$r_B = \widetilde{V}^T B x_+, \qquad \gamma_B = \|B x_+ - \widetilde{V} r_B\|, \qquad v_+ = \frac{B x_+ - \widetilde{V} r_B}{\gamma_A}.$$

CPF-JDGSVD then computes a new approximate GSVD component of (A, B) with respect to \mathcal{U}_{new} , \mathcal{V}_{new} and \mathcal{X}_{new} , and repeat the above process until the convergence criterion (2.6) is achieved. We call iterative solutions of (2.8) the inner iterations and the extractions of the approximate GSVD components with respect to \mathcal{U} , \mathcal{V} and \mathcal{X} the outer iterations.

As has been shown in [15], it suffices to iteratively solve the correction equations approximately with low or modest accuracy and uses an approximate solution to update \mathcal{X} in the above way, in order that the resulting *inexact* CPF-JDGSVD method and its *exact* counterpart with the correction equations solved accurately behave similarly. Precisely, for the correction equation (2.8), we adopt the inner stopping criteria

in [15] and stop the inner iterations when the inner relative residual norm $||r_{in}||$ satisfies

$$||r_{in}|| \le \min\{2c\tilde{\varepsilon}, 0.01\},\$$

where $\tilde{\varepsilon} \in [10^{-4}, 10^{-3}]$ is a user prescribed parameter and c is a constant depending on ρ and the current approximate generalized singular values.

- 3. The harmonic extraction based JDGSVD methods. We shall make use of the principle of the harmonic extraction [31, 33] to propose the CPF-harmonic and IF-harmonic extraction based JDGSVD methods in Section 3.1 and Section 3.2, respectively. They compute new approximate GSVD components of (A, B) with respect to the given left and right searching subspaces \mathcal{U} , \mathcal{V} and \mathcal{X} , and suit better for the computation of interior GSVD components.
- **3.1. The CPF-harmonic extraction approach.** If B has full column rank with some special, e.g., banded, structure, from which the inversion $(B^TB)^{-1}$ can be efficiently applied, we can propose our CPF-harmonic extraction approach to compute a desired approximate GSVD component as follows. For the purpose of derivation, assume that

$$(3.1) B^T B = LL^T$$

is the Cholesky factorization of B^TB with $L \in \mathbb{R}^{n \times n}$ being nonsingular and lower triangular, and define the matrix

$$(3.2) \check{A} = AL^{-T}.$$

We present the following result, which establishes the relationship between the GSVD of (A, B) and the SVD of \check{A} and will be used to propose the CPF-harmonic extraction approach.

Theorem 3.1. Let $(\alpha_*, \beta_*, u_*, v_*, x_*)$ be a GSVD component of the regular matrix pair (A, B) and $\sigma_* = \frac{\alpha_*}{\beta_*}$. Assume that B has full column rank and B^TB has the Cholesky factorization (3.1), and let \check{A} be defined by (3.2) and the vector

$$z_* = \frac{1}{\beta_*} L^T x_*.$$

Then (σ_*, u_*, z_*) is a singular triplet of \check{A} :

$$\check{A}z_* = \sigma_* u_* \qquad and \qquad \check{A}^T u_* = \sigma_* z_*.$$

Proof. It follows from the GSVD (1.2) of (A, B) that $Bx_* = \beta_* v_*$ with $||v_*|| = 1$, meaning that $||Bx_*|| = \beta_*$. Making use of (3.1), we have

$$||z_*|| = \frac{1}{\beta_*} ||L^T x_*|| = \frac{1}{\beta_*} ||B x_*|| = 1.$$

By the definitions (3.2) and (3.3) of \check{A} and z_* , from $Ax_* = \alpha_* u_*$ we obtain

$$\check{A}z_* = \frac{1}{\beta_*}AL^{-T}L^Tx_* = \frac{1}{\beta_*}Ax_* = \frac{\alpha_*}{\beta_*}u_* = \sigma_*u_*,$$

that is, the first relation in (3.4) holds. From the GSVD (1.2), it is straightforward that $A^T u_* = \sigma_* B^T v_* = \frac{\sigma_*}{\beta_*} B^T B x_*$. Making use of this relation and (3.1) gives

$$\check{A}^T u_* = L^{-1} A^T u_* = \frac{\sigma_*}{\beta_*} L^{-1} B^T B x_* = \frac{\sigma_*}{\beta_*} L^T x_* = \sigma_* z_*,$$

which proves the second relation in (3.4).

Theorem 3.1 motivates us to propose our first harmonic extraction approach to compute the singular triplet (σ_*, u_*, z_*) of \check{A} and then recover the desired GSVD component $(\alpha_*, \beta_*, u_*, v_*, x_*)$ of (A, B).

Specifically, take the k-dimensional \mathcal{U} and $\mathcal{Z} = L^T \mathcal{X}$ as the left and right searching subspaces for the left and right singular vectors u_* and z_* of \check{A} , respectively. Then the columns of $\widetilde{Z} = L^T \widetilde{X}$ form a basis of \mathcal{Z} . Mathematically, we seek for positive $\phi > 0$ and vectors $\check{u} \in \mathcal{U}$ and $\check{z} \in \mathcal{Z}$ such that

$$(3.5) \qquad \begin{bmatrix} 0 & \check{A}^T \\ \check{A} & 0 \end{bmatrix} \begin{bmatrix} \check{z} \\ \check{u} \end{bmatrix} - \phi \begin{bmatrix} \check{z} \\ \check{u} \end{bmatrix} \perp \begin{pmatrix} \begin{bmatrix} 0 & \check{A}^T \\ \check{A} & 0 \end{bmatrix} - \tau I \end{pmatrix} \mathcal{R} \begin{pmatrix} \begin{bmatrix} \widetilde{Z} \\ & \widetilde{U} \end{bmatrix} \end{pmatrix}.$$

This is the harmonic extraction approach for the eigenvalue problem of the augmented matrix

$$\begin{bmatrix} 0 & \check{A}^T \\ \check{A} & 0 \end{bmatrix}$$

for the given target $\tau > 0$ [31, 33], where ϕ is a harmonic Ritz value and $[\check{z}^T, \check{u}^T]^T$ is the harmonic Ritz vector with respect to the searching subspace

$$\mathcal{R}\left(\begin{bmatrix} \widetilde{Z} & \\ & \widetilde{U} \end{bmatrix}\right).$$

We pick up the ϕ closest to τ as the approximation to σ_* and take the normalized $\check{z}/\|\check{z}\|$ and $\check{u}/\|\check{u}\|$ as approximations to z_* and u_* , respectively. We will show how to obtain an approximation to x_* afterwards.

Write $\check{z} = \widetilde{Z}\check{d}$ and $\check{u} = \widetilde{U}\check{e}$ with $\check{d} \in \mathbb{R}^k$ and $\check{e} \in \mathbb{R}^k$. Then $\begin{bmatrix} \check{z} \\ \check{u} \end{bmatrix} = \begin{bmatrix} \widetilde{Z} \\ \widetilde{e} \end{bmatrix}$, and requirement (3.5) amounts to the equation

$$\begin{bmatrix} \widetilde{Z}^T & \\ & \widetilde{U}^T \end{bmatrix} \begin{bmatrix} -\tau I & \check{A}^T \\ \check{A} & -\tau I \end{bmatrix} \begin{bmatrix} -\phi I & \check{A}^T \\ \check{A} & -\phi I \end{bmatrix} \begin{bmatrix} \widetilde{Z} & \\ \check{U} \end{bmatrix} \begin{bmatrix} \check{d} \\ \check{e} \end{bmatrix} = 0.$$

Decompose $\phi = \tau + (\phi - \tau)$, and rearrange the above equation. Then we obtain the generalized eigenvalue problem of a 2k-by-2k matrix pair:

$$\begin{bmatrix} \tilde{Z}^T \check{A}^T \check{A} \tilde{Z} + \tau^2 \tilde{Z}^T \tilde{Z} & -2\tau \tilde{Z}^T \check{A}^T \tilde{U} \\ -2\tau \tilde{U}^T \check{A} \tilde{Z} & \tilde{U}^T \check{A} \check{A}^T \tilde{U} + \tau^2 I \end{bmatrix} \begin{bmatrix} \check{d} \\ \check{e} \end{bmatrix} = (\phi - \tau) \begin{bmatrix} -\tau \tilde{Z}^T \tilde{Z} & \tilde{Z}^T \check{A}^T \tilde{U} \\ \tilde{U}^T \check{A} \tilde{Z} & -\tau I \end{bmatrix} \begin{bmatrix} \check{d} \\ \check{e} \end{bmatrix}.$$

By (3.2), $\widetilde{Z} = L^T \widetilde{X}$ and the thin QR factorization of $A\widetilde{X}$ in (2.2), we have

$$\check{A}\widetilde{Z} = A\widetilde{X} = \widetilde{U}R_A,$$

showing that

$$\widetilde{Z}^T \check{A}^T \check{A} \widetilde{Z} = R_A^T R_A$$
 and $\widetilde{Z}^T \check{A}^T \widetilde{U} = R_A^T$.

Moreover, exploiting the Cholesky factorization (3.1) of $B^T B$ and the thin QR factorization of $B\widetilde{X}$ in (2.2), we obtain

$$\begin{split} \widetilde{Z}^T \widetilde{Z} &= \widetilde{X}^T L L^T \widetilde{X} = \widetilde{X}^T B^T B \widetilde{X} = R_B^T R_B, \\ \widetilde{U}^T \widecheck{A} \widecheck{A}^T \widetilde{U} &= \widetilde{U}^T A (L L^T)^{-1} A^T \widetilde{U} = \widetilde{U}^T A (B^T B)^{-1} A^T \widetilde{U}. \end{split}$$

Substituting these two relations into (3.6) yields

$$\begin{aligned} (3.7) \quad \begin{bmatrix} R_A^T R_A + \tau^2 R_B^T R_B & -2\tau R_A^T \\ -2\tau R_A & \widetilde{U}^T A (B^T B)^{-1} A^T \widetilde{U} + \tau^2 I \end{bmatrix} \begin{bmatrix} \widetilde{d} \\ \widecheck{e} \end{bmatrix} \\ &= (\phi - \tau) \begin{bmatrix} -\tau R_B^T R_B & R_A^T \\ R_A & -\tau I \end{bmatrix} \begin{bmatrix} \widecheck{d} \\ \widecheck{e} \end{bmatrix}. \end{aligned}$$

For the brevity of presentation, we will denote the symmetric matrices

$$H_{A,B^{\dagger}} = \widetilde{U}^T A (B^T B)^{-1} A^T \widetilde{U}$$

and

(3.8)
$$G_{c} = \begin{bmatrix} -\tau R_{B}^{T} R_{B} & R_{A}^{T} \\ R_{A} & -\tau I \end{bmatrix}, \qquad H_{c} = \begin{bmatrix} R_{A}^{T} R_{A} + \tau^{2} R_{B}^{T} R_{B} & -2\tau R_{A}^{T} \\ -2\tau R_{A} & H_{A,B^{\dagger}} + \tau^{2} I \end{bmatrix}.$$

In implementations, we compute the generalized eigendecomposition of the symmetric positive definite matrix pair (G_c, H_c) and pick up the largest eigenvalue μ in magnitude and the corresponding unit-length eigenvector $\begin{bmatrix} \vec{q} \end{bmatrix}$. Then the harmonic Ritz approximation to the desired singular triplet $(\sigma_*, \check{u}_*, \check{z}_*)$ of \check{A} is

$$(\phi, \check{u}, \check{z}) = \left(\tau + \frac{1}{\mu}, \frac{\widetilde{U}\check{e}}{\|\check{e}\|}, \frac{\widetilde{Z}\check{d}}{\|\widetilde{Z}\check{d}\|}\right).$$

Since $\check{z} = \frac{\widetilde{Z}\check{d}}{\|\widetilde{Z}\check{d}\|} = \frac{L^T\widetilde{X}\check{d}}{\|L^T\widetilde{X}\check{d}}\|$ is an approximation to the right singular vector z_* of \check{A} , from (3.3) the vector $L^{-T}\check{z} = \widetilde{X}\check{d}$ after some proper normalization is an approximation to the right generalized singular vector x_* of (A,B), which we write as

$$\dot{x} = \frac{1}{\check{\delta}} \widetilde{X} \check{d},$$

where $\check{\delta}$ is a normalizing factor. It is natural to require that the approximate right singular vector \check{x} be (A^TA+B^TB) -norm normalized, i.e., $\check{x}^T(A^TA+B^TB)\check{x}=1$, since the exact x_* satisfies $x_*^T(A^TA+B^TB)x_*=1$ by (1.2). With this normalization, from (3.10), we have

$$1 = \frac{1}{\check{\delta}^2} \check{d}^T \widetilde{X}^T (A^T A + B^T B) \widetilde{X} \check{d} = \frac{1}{\check{\delta}^2} \check{d}^T (R_A^T R_A + R_B^T R_B) \check{d},$$

from which it follows that

(3.11)
$$\check{\delta} = \sqrt{\|R_A \check{d}\|^2 + \|R_B \check{d}\|^2}.$$

Note that the approximate left generalized singular vector \check{u} defined by (3.9) is no longer collinear with $A\check{x}$, as opposed to the collinear \tilde{u} and $A\tilde{x}$ obtained by the standard extraction approach in Section 2. To this end, instead of \check{u} in (3.9), we take new \check{u} and \check{v} defined by

(3.12)
$$\check{u} = \frac{A\check{x}}{\|A\check{x}\|} \quad \text{and} \quad \check{v} = \frac{B\check{x}}{\|B\check{x}\|}$$

as the harmonic Ritz approximations to u_* and v_* , which are colinear with $A\check{x}$ and $B\check{x}$, respectively. Correspondingly, define $\check{e} = R_A\check{d}$ and $\check{f} = R_B\check{d}$. Then by (3.11), the parameter $\check{\delta}$ in (3.10) becomes $\check{\delta} = \sqrt{\|\check{e}\|^2 + \|\check{f}\|^2}$. Moreover, by definition (3.10) of \check{x} and the thin QR factorizations of $A\widetilde{X}$ and $B\widetilde{X}$ in (2.2), we obtain

$$A\check{x} = \frac{1}{\check{\delta}} A \widetilde{X} \check{d} = \frac{1}{\check{\delta}} \widetilde{U} R_A \check{d} = \frac{1}{\check{\delta}} \widetilde{U} \check{e},$$

$$B\check{x} = \frac{1}{\check{\delta}} B \widetilde{X} \check{d} = \frac{1}{\check{\delta}} \widetilde{V} R_B \check{d} = \frac{1}{\check{\delta}} \widetilde{V} \check{f}.$$

Using them, we can efficiently compute the approximate generalized singular vectors

(3.13)
$$\check{u} = \frac{A\check{x}}{\|A\check{x}\|} = \frac{\widetilde{U}\check{e}}{\|\check{e}\|} \quad \text{and} \quad \check{v} = \frac{B\check{x}}{\|B\check{x}\|} = \frac{\widetilde{V}\check{f}}{\|\check{f}\|}$$

without forming products of the vector \check{x} with the large A and B.

As for the approximate generalized singular value ϕ in (3.9), we replace it by the Rayleigh quotient $\check{\theta} = \frac{\check{\alpha}}{\check{\beta}}$ of (A,B) with respect to the approximate left and right generalized singular vectors \check{u} and \check{v} , \check{x} , where

(3.14)
$$\check{\alpha} = \check{u}^T A \check{x} = \frac{\|\check{e}\|}{\check{\delta}} \quad \text{and} \quad \check{\beta} = \check{v}^T B \check{x} = \frac{\|\check{f}\|}{\check{\delta}}.$$

The reason is that $\check{\theta}$ is a better approximation to σ_* than the harmonic Ritz value ϕ in the sense that

$$(3.15) ||(A^T A - \check{\theta}^2 B^T B) \check{x}||_{(B^T B)^{-1}} \le ||(A^T A - \phi^2 B^T B) \check{x}||_{(B^T B)^{-1}}.$$

We remark that the residual of $(\check{\alpha}, \check{\beta}, \check{u}, \check{v}, \check{x})$ can be defined similarly to (2.5), and a stopping criterion similar to (2.6) can be used.

The CPF-harmonic extraction approach does not need to form the cross product matrices A^TA or B^TB explicitly. To distinguish from the approximation obtained by the IF-harmonic extraction approach to be proposed in the next subsection, we call $(\check{\alpha}, \check{\beta}, \check{u}, \check{v}, \check{x})$ the CPF-harmonic Ritz approximation to $(\alpha_*, \beta_*, u_*, v_*, x_*)$ with respect to the left and right searching subspaces \mathcal{U}, \mathcal{V} and \mathcal{X} , where $(\check{\alpha}, \check{\beta})$ or $\check{\theta}$ is the CPF-harmonic Ritz value, and \check{u}, \check{v} and \check{x} are the left and right CPF-harmonic Ritz vectors, respectively. Particularly, if we expand \mathcal{U}, \mathcal{V} and \mathcal{X} in a similar manner to that described in Section 2, the resulting method is called the CPF-harmonic JDGSVD method, abbreviated as the CPF-HJDGSVD method.

From (3.7), we can efficiently update the projected matrix pair (G_c, H_c) as the subspaces are expanded. At each expansion step, one needs to solve the large symmetric positive definite linear equations with the coefficient matrix B^TB and the multiple right-hand sides $A^T\widetilde{U}$. This can be done efficiently in parallel whenever the Cholesky

factorization (3.1) of B^TB can be computed efficiently, which is the case for some structured B, e.g., banded structure.

However, for a general large and sparse B, the calculation of the Cholesky factorization (3.1) of B^TB may be costly and even computationally infeasible. In this case, we can compute $(B^TB)^{-1}A^T\widetilde{U}$ using the Conjugate Gradient (CG) method for each column of $A^T\widetilde{U}$. For B well conditioned, the CG method converges fast.

Finally, we remark that, when A is of full column rank, the CPF-harmonic extraction approach proposed above can be directly applied to the matrix pair (B, A), whose GSVD components are $(\beta_i, \alpha_i, v_i, u_i, x_i)$, $i = 1, \ldots, q$.

3.2. The IF-harmonic extraction approach. As is clear from the previous subsection, CPF-HJDGSVD requires that the symmetric B^TB be positive definite, namely, B is square or rectangular and has full column rank. If the direct application of $(B^TB)^{-1}$ is unaffordable or the CG method converges slowly, then the CPF-harmonic extraction approach is costly. Alternatively, we will propose an inverse-free (IF) harmonic extraction approach that avoids this difficulty and removes the above restriction on B.

Given the right searching subspace \mathcal{X} , the IF-harmonic extraction approach seeks for an approximate generalized singular value $\varphi > 0$ and an approximate right generalized singular vector $\hat{x} \in \mathcal{X}$ with $\|\hat{x}\|_{A^TA+B^TB} = 1$ such that

$$(3.16) (A^T A - \varphi^2 B^T B) \hat{x} \perp (A^T A - \tau^2 B^T B) \mathcal{X},$$

namely, the residual of (φ^2, \hat{x}) as an approximate generalized eigenpair of the matrix pair (A^TA, B^TB) is orthogonal to the subspace $(A^TA - \tau^2B^TB)\mathcal{X}$. This is precisely the harmonic Rayleigh–Ritz projection of (A^TA, B^TB) onto \mathcal{X} with respect to the target τ^2 , and the k pairs (φ^2, \hat{x}) are the harmonic Ritz approximations of (A^TA, B^TB) with respect to \mathcal{X} for the given τ^2 . One selects the positive φ closest to τ and the corresponding \hat{x} as approximations to the desired generalized singular value σ closest to τ and the corresponding right generalized singular vector x.

Since the columns of $(A^TA - \tau^2B^TB)\widetilde{X}$ span the subspace $(A^TA - \tau^2B^TB)\mathcal{X}$, requirement (3.16) is equivalent to

$$\widetilde{X}^T (A^T A - \tau^2 B^T B) (A^T A - \varphi^2 B^T B) \widetilde{X} \hat{d} = 0$$
 with $\hat{x} = \frac{1}{\hat{\delta}} \widetilde{X} \hat{d}$,

where $\hat{\delta}$ is a normalizing factor such that $\|\hat{x}\|_{A^TA+B^TB} = 1$.

Writing $\varphi^2 = \tau^2 + (\varphi^2 - \tau^2)$ and rearranging the above equation, we obtain

$$(3.17) \qquad \widetilde{X}^T (A^T A - \tau^2 B^T B)^2 \widetilde{X} \hat{d} = (\varphi^2 - \tau^2) \widetilde{X}^T (A^T A - \tau^2 B^T B) B^T B \widetilde{X} \hat{d},$$

that is, $\mu = \varphi^2 - \tau^2$ is a generalized eigenvalue of the matrix pair (H_τ, G_τ) and \hat{d} is the corresponding normalized generalized eigenvector, where

$$(3.18) \ G_{\tau} = \widetilde{X}^T (A^T A - \tau^2 B^T B) B^T B \widetilde{X} \qquad \text{and} \qquad H_{\tau} = \widetilde{X}^T (A^T A - \tau^2 B^T B)^2 \widetilde{X}.$$

We compute the generalized eigendecomposition of (G_{τ}, H_{τ}) , pick up its largest generalized eigenvalue $\nu = \frac{1}{\mu}$ in magnitude, and take $\varphi = \sqrt{\tau^2 + \frac{1}{\nu}}$ as an approximation to σ_* . Correspondingly, the harmonic Ritz pair to approximate (σ_*, x_*) is

(3.19)
$$(\varphi, \hat{x}) = \left(\sqrt{\tau^2 + \frac{1}{\nu}}, \frac{1}{\hat{\delta}} \widetilde{X} \hat{d}\right),$$

where \hat{d} is the generalized eigenvector of (G_{τ}, H_{τ}) corresponding to the eigenvalue ν . As for the normalizing factor $\hat{\delta}$, by the requirement that $\|\hat{x}\|_{A^TA+B^TB}=1$, following the same derivations as in Section 3.1, we have

(3.20)
$$\hat{\delta} = \sqrt{\|\hat{e}\|^2 + \|\hat{f}\|^2}$$
 with $\hat{e} = R_A \hat{d}$ and $\hat{f} = R_B \hat{d}$,

where R_A and R_B are defined by (2.2). Analogously to that done in Section 3.1, rather than using the harmonic Ritz value φ to approximate σ_* , we recompute a new and better approximate generalized singular value and the corresponding left generalized singular vectors by

(3.21)
$$\hat{\alpha} = ||A\hat{x}||, \quad \hat{\beta} = ||B\hat{x}|| \quad \text{and} \quad \hat{u} = \frac{A\hat{x}}{||A\hat{x}||}, \quad \hat{v} = \frac{B\hat{x}}{||B\hat{x}||}.$$

Since the new approximate generalized singular value $\hat{\theta} = \frac{\hat{\alpha}}{\hat{\beta}}$ is the square root of the Rayleigh quotient of the matrix pair (A^TA, B^TB) with respect to \hat{x} , as an approximation to σ_* , it is more accurate than φ in (3.19) in the sense of (3.15) when the CPF-harmonic approximations \check{x} , $\check{\theta}$ and φ are replaced by the IF-harmonic ones \hat{x} , $\hat{\theta}$ and φ , respectively.

It is straightforward to verify that $(\hat{\alpha}, \hat{\beta}, \hat{u}, \hat{v}, \hat{x})$ in (3.21) satisfies $A\hat{x} = \hat{\alpha}u$ and $B\hat{x} = \hat{\beta}\hat{v}$ with $\|\hat{u}\| = \|\hat{v}\| = 1$ and $\hat{\alpha}^2 + \hat{\beta}^2 = 1$. By (2.2), (3.20) and (3.21), it is easily shown that

$$\hat{\alpha} = \frac{\|\hat{e}\|}{\hat{\delta}}, \qquad \hat{\beta} = \frac{\|\hat{f}\|}{\hat{\delta}} \qquad \text{and} \qquad \hat{u} = \frac{\widetilde{U}\hat{e}}{\|\hat{e}\|}, \qquad \hat{v} = \frac{\widetilde{V}\hat{f}}{\|\hat{f}\|}.$$

Therefore, compared with (3.21), we can exploit formula (3.22) to compute $\hat{\alpha}, \hat{\beta}$ and \hat{u}, \hat{v} more efficiently without using A and B to form matrix-vector products. We call $(\hat{\alpha}, \hat{\beta}, \hat{u}, \hat{v}, \hat{x})$ the IF-harmonic Ritz approximation to $(\alpha_*, \beta_*, u_*, v_*, x_*)$ with respect to the left and right searching subspaces \mathcal{U}, \mathcal{V} and \mathcal{X} , where the pair $(\hat{\alpha}, \hat{\beta})$ or $\hat{\theta} = \frac{\hat{\alpha}}{\hat{\beta}}$ is the IF-harmonic Ritz value, and \hat{u}, \hat{v} and \hat{x} are the left and right IF-harmonic Ritz vectors, respectively. Particularly, when expanding \mathcal{U}, \mathcal{V} and \mathcal{X} in a similar manner to that described in Section 2, the resulting method is called the IF-harmonic JDGSVD method, abbreviated as the IF-HJDGSVD method.

Based on the way that $(\hat{\alpha}, \hat{\beta}, \hat{u}, \hat{v}, \hat{x})$ is computed, the associated residual and stopping criterion are defined as (2.5) and designed as (2.6), respectively.

In computations, as \mathcal{U}, \mathcal{V} and \mathcal{X} are expanded, we first update the intermediate matrices

$$(3.23) \qquad H_A = \widetilde{X}^T (A^T A)^2 \widetilde{X}, \quad H_B = \widetilde{X}^T (B^T B)^2 \widetilde{X}, \quad H_{A,B} = \widetilde{X}^T A^T A B^T B \widetilde{X}$$

efficiently and then form the matrices

(3.24)
$$G_{\tau} = H_{A,B} - \tau^2 H_B$$
 and $H_{\tau} = H_A + \tau^4 H_B - \tau^2 (H_{A,B}^T + H_{A,B}).$

Compared with the CPF-harmonic extraction, the IF-harmonic extraction does not involve $(B^TB)^{-1}$. Note that it uses B^TB and A^TA explicitly when forming the matrices G_{τ} and H_{τ} in (3.18). Fortunately, provided that the desired σ_* is not very small, then σ_*^2 is a well conditioned eigenvalue of (A^TA, B^TB) and $\hat{\theta}$ is an approximation to σ_* with the accuracy $\|(A^TA - \hat{\theta}^2B^TB)\hat{x}\|$ [32, Sect. 3, Chap. XI].

- 4. Thick-restart JDGSVD type algorithms with deflation and purgation. As the subspace dimension k increases, the computational complexity of the proposed JDGSVD type algorithms will become prohibitive. For a maximum number $k = k_{\text{max}}$ allowed, if the algorithms do not yet converge, then it is necessary to restart them. In this section, we show how to effectively and efficiently restart CPF-HJDGSVD and IF-HJDGSVD proposed in Section 3, and how to introduce some efficient novel deflation and purgation techniques into them to compute more than one, i.e., $\ell > 1$, GSVD components of (A, B).
- 4.1. Thick-restart. We adopt a commonly used thick-restart technique, which was initially advocated in [30] and has been popularized in a number of papers, e.g., [14, 15, 30, 35, 36]. Adapting it to our case, we take three new initial searching subspaces to be certain k_{\min} -dimensional subspaces of the left and right searching subspaces at the current cycle, which aim to contain as much information as possible on the desired left and right generalized singular vectors and their few neighbors. Then we continue to expand the subspaces in the regular way described in Sections 2–3, and compute new approximate GSVD components with respect to the expanded subspaces. We check the convergence at each step, and if converged, stop; otherwise expand the subspaces until the subspace dimension reaches k_{\max} . Proceed in this way until the desired GSVD component is found. In what follows we describe how to efficiently implement thick-restart in our GSVD context, which turns out to be involved and is not as direct as in the context of the standard eigenvalue problem and SVD problem.

At the current extraction phase, either CPF-HJDGSVD or IF-HJDGSVD has computed k_{\min} approximate right generalized singular vectors, denoted by $\tilde{x}_i = \widetilde{X} d_i$ in a unified form, corresponding to the k_{\min} approximate generalized singular values closest to τ , where \tilde{x}_1 is used to approximate the desired x_* . Write $\widetilde{X}_1 = [\tilde{x}_1, \dots, \tilde{x}_{k_{\min}}]$ and $D_1 = [d_1, \dots, d_{k_{\min}}]$, and take the new initial right searching subspace

$$\mathcal{X}_{\text{new}} = \text{span}\{\widetilde{X}_1\} = \text{span}\{\widetilde{X}D_1\}.$$

Compute the thin QR factorization of D_1 to obtain its Q-factor $Q_d \in \mathbb{R}^{k_{\text{max}} \times k_{\text{min}}}$. Then the columns of

$$\widetilde{X}_{\text{new}} = \widetilde{X}Q_d$$

form an orthonormal basis of \mathcal{X}_{new} . Correspondingly, we take the new initial left subspaces $\mathcal{U}_{\text{new}} = A\mathcal{X}_{\text{new}}$ and $\mathcal{V}_{\text{new}} = B\mathcal{X}_{\text{new}}$. Notice that

$$A\widetilde{X}_{\text{new}} = A\widetilde{X}Q_d = \widetilde{U}R_AQ_d$$
 and $B\widetilde{X}_{\text{new}} = B\widetilde{X}Q_d = \widetilde{V}R_BQ_d$.

We compute the thin QR factorizations of the small matrices R_AQ_d and R_BQ_d :

$$R_A Q_d = Q_e R_{A,\text{new}}$$
 and $R_B Q_d = Q_f R_{B,\text{new}}$,

where $Q_e, Q_f \in \mathbb{R}^{k_{\text{max}} \times k_{\text{min}}}$ are orthonormal, and $R_{A,\text{new}}$ and $R_{B,\text{new}} \in \mathbb{R}^{k_{\text{min}} \times k_{\text{min}}}$ are upper triangular. Then the columns of

$$\widetilde{U}_{
m new} = \widetilde{U}Q_e$$
 and $\widetilde{V}_{
m new} = \widetilde{V}Q_f$

form orthonormal bases of \mathcal{U}_{new} and \mathcal{V}_{new} , and $R_{A,\text{new}}$ and $R_{B,\text{new}}$ are the R-factors of $A\widetilde{X}_{\text{new}} = \widetilde{U}_{\text{new}}R_{A,\text{new}}$ and $B\widetilde{X}_{\text{new}} = \widetilde{V}_{\text{new}}R_{B,\text{new}}$, respectively.

For the CPF-harmonic extraction, we need to update the projection matrices $G_{\rm c}$ and $H_{\rm c}$ defined by (3.8). Concretely, we compute $G_{\rm c,new}$ and the (1,1)-, (1,2)-and (2,1)-block submatrices of $H_{\rm c,new}$ by using $R_{A,\rm new}$ and $R_{B,\rm new}$. The (2,2)-block submatrix $H_{\rm c2,new} = H_{A,B^{\dagger},\rm new} + \tau^2 I$ of $H_{\rm c,new}$ is updated efficiently without involving $(B^TB)^{-1}$:

$$(4.2) H_{A,B^{\dagger},\text{new}} = \widetilde{U}_{\text{new}}^T A (B^T B)^{-1} A^T \widetilde{U}_{\text{new}} = Q_e^T H_{A,B^{\dagger}} Q_e$$

where $H_{A,B^{\dagger}} = \widetilde{U}^T A (B^T B)^{-1} A^T \widetilde{U}$ is part of the (2,2)-block submatrix of H_c . For the IF-harmonic extraction, we efficiently update the intermediate matrices H_A , H_B and $H_{A,B}$ in (3.23) by

$$H_{A,\text{new}} = Q_d^T H_A Q_d, \qquad H_{B,\text{new}} = Q_d^T H_B Q_d, \qquad H_{A,B,\text{new}} = Q_d^T H_{A,B} Q_d.$$

4.2. Deflation and purgation. If the GSVD components $(\alpha_i, \beta_i, u_i, v_i, x_i)$, $i = 1, \ldots, \ell$ of (A, B) are required with $\sigma_i = \frac{\alpha_i}{\beta_i}$ labeled as in (1.3), we can adapt the efficient deflation and purgation techniques in [15] to our JDGSVD algorithms.

Assume that the j approximate GSVD components $(\alpha_{i,c}, \beta_{i,c}, u_{i,c}, v_{i,c}, x_{i,c})$ have converged to the desired GSVD components $(\alpha_i, \beta_i, u_i, v_i, x_i)$ with

$$(4.3) ||r_i|| = ||\beta_{i,c}A^T u_{i,c} - \alpha_{i,c}B^T v_{i,c}|| \le (\beta_{i,c}||A||_1 + \alpha_{i,c}||B||_1) \cdot tol, \qquad i = 1, \dots, j$$

Write $C_c = \text{diag}\{\alpha_{1,c}, \ldots, \alpha_{j,c}\}$, $S_c = \text{diag}\{\beta_{1,c}, \ldots, \beta_{j,c}\}$ and $U_c = [u_{1,c}, \ldots, u_{j,c}]$, $V_c = [v_{1,c}, \ldots, v_{j,c}]$, $X_c = [x_{1,c}, \ldots, x_{j,c}]$. Then $(C_c, S_c, U_c, V_c, X_c)$ is a converged approximate partial GSVD of (A, B) that satisfies

$$AX_c = U_cC_c, \qquad BX_c = V_cS_c, \qquad C_c^2 + S_c^2 = I_j$$

and

$$||R_c||_F = ||A^T U_c S_c - B^T V_c C_c||_F \le \sqrt{j(||A||_1^2 + ||B||_1^2)} \cdot tol.$$

Proposition 4.1 of [15] proves that if tol = 0 in (4.3) then the exact nontrivial GSVD components of the modified matrix pair

(4.4)
$$(A(I - X_c Y_c^T), B(I - X_c Y_c^T))$$
 with $Y_c = (A^T A + B^T B)X_c$

are $(\alpha_i, \beta_i, u_i, v_i, x_i)$, i = j + 1, ..., q, where Y_c satisfies $X_c^T Y_c = I_j$. Therefore, we can apply either CPF-HJDGSVD or IF-HJDGSVD to the pair (4.4), and compute the next desired GSVD component $(\alpha_*, \beta_*, u_*, v_*, x_*) := (\alpha_{j+1}, \beta_{j+1}, u_{j+1}, v_{j+1}, x_{j+1})$.

To this end, we require that the converged X_c and Y_c be bi-orthogonal, i.e., $X_c^T Y_c = I$. Moreover, as the right searching subspace \mathcal{X} is expanded, we require that \mathcal{X} be always $(A^T A + B^T B)$ -orthogonal to the converged approximate right generalized singular vectors $x_{1,c}, \ldots, x_{j,c}$, i.e., $\widetilde{X}^T Y_c = \mathbf{0}$. Such an orthogonality can be guaranteed in computations, as shown below.

Assume that $X_c^T Y_c = I_j$ and $\widetilde{X}^T \perp Y_c$. At the extraction phase, we use the CPF-harmonic or IF-harmonic extraction to obtain an approximate GSVD component (α, β, u, v, x) of (A, B). If (α, β, u, v, x) has not yet converged, we construct $X_p = [X_c, x]$ and $Y_p = [Y_c, y]$ with $y = (A^T A + B^T B)x = \alpha A^T u + \beta B^T v$. Then it follows from $X_c^T Y_c = I_j$ and $x \perp Y_c$ that $X_c^T y = Y_c^T x = \mathbf{0}$, $x^T y = 1$ and $x_p^T Y_p = I_{j+1}$. Therefore, $I - Y_p X_p^T$ is an oblique projector. At the subspace expansion phase, instead

of (2.8), we use an iterative solver, e.g., the MINRES method [29], to approximately solve the modified symmetric correction equation

(4.5)
$$(I - Y_p X_p^T)(A^T A - \rho^2 B^T B)(I - X_p Y_p^T)t = -(I - Y_p X_p^T)r$$
 for $t \perp Y_p$

with r being the residual (2.5) of (α, β, u, v, x) and $\rho = \tau$ or $\frac{\alpha}{\beta}$. Having found an approximate solution $\tilde{t} \perp Y_p$, we orthonormalize it against \tilde{X} to obtain the expansion vector x_+ and update \tilde{X} by (2.10). By assumption and (4.5), both \tilde{X} and \tilde{t} are orthogonal to Y_c , which makes the expansion vector x_+ and the expanded right searching subspace \mathcal{X} orthogonal to Y_c .

If (α, β, u, v, x) has already converged, we add it to the converged partial GSVD $(C_c, S_c, U_c, V_c, X_c)$ and set j := j + 1. By assumption, the old X_c and Y_c are bi-orthogonal. Since the added x is orthogonal to the old Y_c , it is known that the new X_c and Y_c are also bi-orthogonal. Proceed in this way until all the ℓ desired GSVD components of (A, B) are found.

Remarkably, when (α, β, u, v, x) has converged, the current searching subspaces usually contain reasonably good information on the next desired GSVD component. In order to make full use of such available information when computing the next $(\alpha_*, \beta_*, u_*, v_*, x_*)$, the authors in [14, 15] have proposed an effective and efficient purgation strategy. It can be adapted to our current context straightforwardly: We purge the newly converged $x = \widetilde{X}d$ from the current \mathcal{X} and take the reduced subspace \mathcal{X}_{new} as the initial right searching subspace for computing the next desired GSVD component of (A, B). To achieve this, we compute the QR factorization of the $k \times 1$ matrix $d' = (R_A^T R_A + R_B^T R_B)d$ to obtain its Q-factor $\left[\frac{d'}{\|d'\|}, Q_D\right]$ such that the columns of $Q_D \in \mathbb{R}^{k \times (k-1)}$ form an orthonormal basis of the orthogonal completement subspace of span $\{d'\}$. Then the columns of

$$\widetilde{X}_{\text{new}} = \widetilde{X} Q_D$$

form an orthonormal basis of \mathcal{X}_{new} , and $\widetilde{X}_{\text{new}}$ is orthogonal to $Y_{c,\text{new}} = [Y_c, y]$ with $y = (A^T A + B^T B)x$ because $\widetilde{X}_{\text{new}}^T Y_c = \mathbf{0}$ and

$$\widetilde{X}_{\mathrm{new}}^T y = Q_D^T \widetilde{X}^T (A^T A + B^T B) \widetilde{X} d = Q_D^T (R_A^T R_A + R_B^T R_B) d = Q_D^T d' = \mathbf{0}.$$

Therefore, provided that Q_d in (4.1) is replaced by Q_D , just as done in Section 4.1, we can efficiently construct orthonormal base of the new initial searching left and right subspaces \mathcal{U}_{new} , \mathcal{V}_{new} and \mathcal{X}_{new} . Therefore, the purgation can be done with very little cost. We then continue to expand the subspaces in a regular way until their dimensions reach k_{max} .

5. Numerical experiments. In this section, we report numerical experiments on several problems to illustrate the performance of the two harmonic extraction based algorithms CPF-HJDGSVD, IF-HJDGSVD and the standard extraction based algorithm CPF-JDGSVD in [15], and make a comparison of them. All the numerical experiments were performed on an Intel Core (TM) i9-10885H CPU 2.40 GHz with 64 GB RAM using the Matlab R2021a with the machine precision $\epsilon_{\rm mach} = 2.22 \times 10^{-16}$ under the Miscrosoft Windows 10 64-bit system.

Table 1 lists all the test problems together with some of their basic properties, where the matrices A or their transpose(s) are sparse matrices from [8] with $m \ge n$,

A	B	m	p	n	nnz	$\kappa(\left[\begin{smallmatrix} A \\ B \end{smallmatrix} ight])$	$\sigma_{ m max}$	σ_{\min}
nd3k	T	9000	9000	9000	3306688	9.33e + 1	1.16e + 2	1.77e-6
viscoplastic1	T	4326	4326	4326	74142	7.39e + 1	5.26e + 1	1.51e-4
rajat03	T	7602	7602	7602	55457	5.10e + 2	2.65e + 2	8.07e-6
$\mathrm{lp}_\mathrm{bnl}2^T$	T	4486	2324	2324	21966	1.93e + 2	1.10e + 2	1.20e-2
Hamrle2	T	5952	5952	5952	40016	1.04e + 2	7.29e + 1	4.12e-4
$\mathrm{jendrec1}^T$	T	4228	2109	2109	95933	8.95e + 2	1.86e + 3	7.86e-1
grid2	L_1	3296	3295	3296	19454	7.54e + 1	1.93e + 3	3.32e-17
dw1024	L_1	2048	2047	2048	14208	8.03	5.25e + 2	2.55e-4
$r05^T$	L_1	9690	5189	5190	114523	$6.24e{+1}$	1.19e + 4	2.91e-1
$p05^T$	L_1	9590	5089	5090	69223	4.40e + 1	9.77e + 3	2.91e-1
bibd_81_2	L_2	3240	3238	3240	12954	4.12	4.69e + 5	2.50e-1
benzene	L_2	8219	8217	8219	267320	5.58e + 2	1.60e + 7	2.89e-1
blckhole	L_2	2132	2130	2132	21262	3.64e + 1	1.32e + 6	6.90e-4

Table 1
Basic properties of the test matrix pairs.

the matrices B are taken to be (i) the symmetric tridiagonal Toeplitz matrices T with p = n whose diagonal and subdiagonal elements are 3 and 1, respectively, and (ii)

$$L_1 = \begin{bmatrix} 1 & -1 & & & \\ & \ddots & \ddots & & \\ & & 1 & -1 \end{bmatrix} \quad \text{and} \quad L_2 = \begin{bmatrix} -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \end{bmatrix},$$

which are the scaled discrete approximations of the first and second order derivative operators in dimension one with p = n - 1 and p = n - 2, respectively, nnz denotes the total numbers of the nonzero elements in A and B, and σ_{\max} and σ_{\min} denote the largest and smallest nontrivial generalized singular values of (A, B), respectively. We mention that, for those matrix pairs (A, B) with B = T, all the generalized singular values of (A, B) are nontrivial ones and, for the matrix pairs (A, B) with $B = L_1$ and L_2 , there are one and two infinite generalized singular values, respectively.

For the three algorithms under consideration, we take the vectors ones(n, 1) and mod(1:n,4) and normalize them to form one dimensional right searching subspaces for (A, B) with B = T and $B = L_i$, i = 1, 2, respectively, where ones and mod are the Matlab built-in functions. When the dimensions of \mathcal{X} , \mathcal{U} and \mathcal{V} reach the maximum number $k_{\text{max}} = 30$ but the algorithms do not converge, we use the corresponding thick-restart algorithms by taking $k_{\min} = 3$. An approximate GSVD component is claimed to have converged if its relative residual norm satisfies (2.6) with $tol = 10^{-8}$. We stop the algorithms if all the ℓ desired GSVD components have been computed successfully or the total $K_{\text{max}} = n$ outer iterations have been used. For the correction equation (2.8), we first take $\rho = \tau$ and then switch to $\rho = \theta$ if the outer residual norm satisfies (2.9) with $fixtol = 10^{-4}$. We take zero vectors as initial solution guesses for the inner iterations and use the Matlab built-in function minres to solve the correction equation (2.8) or (4.5) until the inner relative residual norm meets (2.11) with the stopping criterion $\tilde{\varepsilon} = 10^{-4}$. We comment that, as our extensive experience has demonstrated, preconditioning the correction equations by ILU type factorizations [29] has turned out to be ineffective and does not reduce the inner iterations for most of the test problems. The ineffectiveness is due to the (high) indefiniteness of correction equations. Therefore, we report only the results using the MINRES method

without preconditioning.

In all the tables, for the ease of presentation, we further abbreviate the CPF-JDGSVD, CPF-HJDGSVD and IF-HJDGSVD algorithms as CPF, CPFH and IFH, respectively. We denote by I_{out} and I_{in} the total numbers of outer and inner iterations that an underlying JDGSVD algorithm uses to achieve the convergence, respectively, and by T_{cpu} the total CPU time in seconds counted by the Matlab built-in commands tic and toc.

Example 5.1. We compute one GSVD component of (A, B) = (nd3k, T) associated with the generalized singular value closest to the target $\tau = 10$ that is highly clustered with some other ones of (A, B).

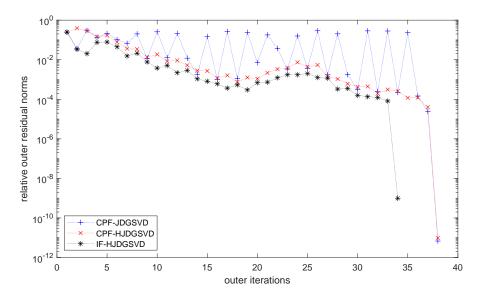


Fig. 1. Computing one GSVD component of (A, B) = (nd3k, T) with $\tau = 10$.

For the matrix pairs (A, B) in this and the next two examples, the matrices B = T's are well conditioned, and their Cholesky factorizations can be cheaply computed at the cost of $\mathcal{O}(n)$ flops, so that each matrix-vector product with B^{-1} can be implemented using $\mathcal{O}(n)$ flops. Therefore, at the expansion phase of each step of CPF-HJDGSVD, we use the Matlab recommended command \setminus to carry out B^{-1} -vector products and update the matrix $H_{A,B^{\dagger}}$ in (3.8). Purely for the experimental purpose and the illustration of the truly convergence behavior, when solving the inner linear systems (2.8) involved in the JDGSVD type algorithms, we compute the LU factorizations of $A^TA - \rho^2B^TB$ and use them to solve the linear systems. That is, we solve all the correction equations accurately in finite precision arithmetic. We will demonstrate how the CPF-harmonic and IF-harmonic extraction approaches behave. Figure 1 depicts the outer convergence curves of the three JDGSVD type algorithms.

As can be seen from Figure 1, compared with CPF-JDGSVD, the two harmonic JDGSVD algorithms have smoother outer convergence behavior, and IF-HJDGSVD uses four fewer outer iterations to reach the convergence than CPF-JDGSVD and CPF-HJDGSVD. This illustrates the advantage of IF-HJDGSVD over CPF-JDGSVD and CPF-HJDGSVD. Of CPF-JDGSVD and CPF-HJDGSVD, although they use the same number of outer iterations to converge, CPF-HJDGSVD should be favorable because of its much more regular convergence behavior.

Example 5.2. We compute one GSVD component of (A, B) = (viscoplastic1, T) with the generalized singular value closest to a small target $\tau = 6.7e - 2$ being clustered with some other ones of (A, B). We should notice that τ is fairly near to the left-end point $\sigma_{\min} = 1.51e - 4$ of the generalized singular spectrum of (A, B). This implies that the desired generalized singular vectors and the correction equations (2.8) are ill conditioned, causing that minres converges slowly.

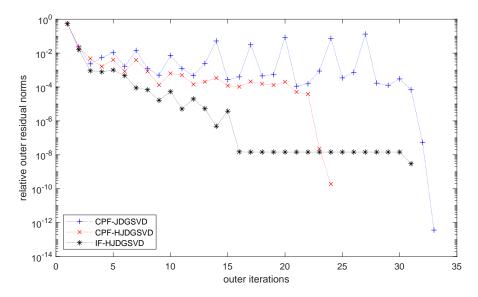


Fig. 2. Computing one GSVD component of (A, B) = (viscoplastic1, T) with $\tau = 6.7e - 2$.

We draw the outer convergence curves of the three JDGSVD type algorithms in Figure 2. As the figure shows, both CPF-HJDGSVD and IF-HJDGSVD converge much more regularly than CPF-JDGSVD. Specifically, IF-HJDGSVD converges much faster than CPF-JDGSVD in the first sixteen outer iterations, and it has already reached the level of $\mathcal{O}(10^{-8})$ at iteration 16. Although it stagnates for the next several outer iterations, IF-HJDGSVD manages to converge two outer iterations more early than CPF-JDGSVD. On the other hand, CPF-HJDGSVD converges steadily in the first twenty-two outer iterations, and it then drops sharply and achieves the convergence criterion in the next two outer iterations. As the results indicate, CPF-HJDGSVD uses seven and nine fewer outer iterations than CPF-JDGSVD and IF-HJDGSVD, respectively.

Obviously, for this problem, both CPF-HJDGSVD and IF-HJDGSVD performs better than CPF-JDGSVD. Of the two harmonic algorithms, CPF-HJDGSVD is favorable for its faster overall convergence.

Example 5.3. We compute ten GSVD components of the matrix pairs $(A_1, B_1) = (\text{rajat03}, T), (A_2, B_2) = (\text{lp-bnl2}^T, T), (A_3, B_3) = (\text{Hamrle2}, T) \text{ and } (A_4, B_4) = (\text{jendrec1}^T, T) \text{ with the generalized singular values closest to the targets } \tau_1 = 50, \tau_2 = 17, \tau_3 = 8 \text{ and } \tau_4 = 6.3, \text{ respectively.}$ The desired generalized singular values of (A_1, B_1) and (A_2, B_2) are the largest ones, which are fairly isolated one another, and those of (A_3, B_3) and (A_4, B_4) are highly clustered interior ones. In the expansion phase of the three algorithms, we use minres without preconditioning to solve all the correction equations.

Figures 3-4 depict the convergence curves of the three JDGSVD algorithms for

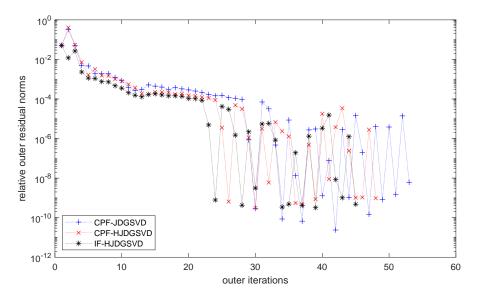


Fig. 3. Computing ten GSVD components of (A, B) = (rajat03, T) with $\tau = 50$.

computing the ten desired GSVD components of (A_1, B_1) and (A_2, B_2) , and Table 2 displays the results on the four test problems.

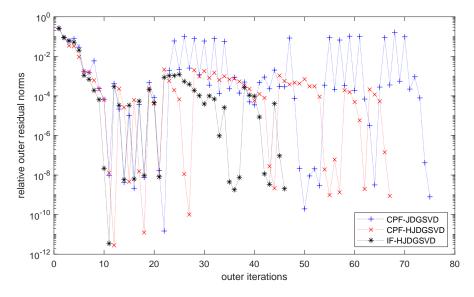


Fig. 4. Computing ten GSVD components of $(A, B) = (lp_bnl2^T, T)$ with $\tau = 17$.

For (A_1, B_1) and (A_2, B_2) , we can observe from the figures and Table 2 that, regarding the outer convergence, CPF-HJDGSVD and especially IF-HJDGSVD outperform CPF-JDGSVD as they use a little bit fewer and substantially fewer outer iterations than the latter for (A_1, B_1) and (A_2, B_2) , respectively. Specifically, for (A_2, B_2) , we see from Figure 4 that the two harmonic algorithms CPF-HJDGSVD and IF-HJDGSVD have much smoother and faster outer convergence. We must remind the reader that, for $\ell=10$, each JDGSVD algorithm has ten convergence stages,

A	Algorithm	I_{out}	I_{in}	T_{cpu}
	CPF	53	14695	3.70
rajat03	CPFH	48	13082	3.48
	IFH	45	13207	3.55
	CPF	75	4971	0.49
lp_bnl2^T	CPFH	67	4609	0.48
	$_{ m IFH}$	46	4477	0.42
	CPF	100	17210	3.50
Hamrle2	CPFH	113	16330	3.60
	$_{ m IFH}$	72	17214	3.69
	CPF	102	13382	2.06
$\mathrm{jendrec1}^T$	CPFH	62	9469	1.53
•	$_{ m IFH}$	42	8848	1.31

Table 2
Results on the test matrix pairs in Example 5.3

which denote the one by one convergence processes of the desired ten GSVD components. In the meantime, we also see from Table 2 that, regarding the overall efficiency, CPF-HJDGSVD and IF-HJDGSVD outperform CPF-JDGSVD in terms of total inner iterations and total CPU time.

For (A_3, B_3) , since the desired generalized singular values are highly clustered, the corresponding left and right generalized singular vectors are ill conditioned. As a result, it may be hard to compute the desired GSVD components using the standard and harmonic JDGSVD algorithms [18]. We observe quite irregular convergence behavior and sharp oscillations of CPF-JDGSVD and CPF-HJDGSVD, while IF-HJDGSVD converges much more smoothly and uses significantly fewer outer iterations, compared with CPF-JDGSVD and CPF-HJDGSVD, as shown in Table 2. Therefore, IF-HJDGSVD is preferable for this problem.

For the matrix pair (A_4, B_4) , the three JDGSVD algorithms succeed in computing all the desired GSVD components. Among them, CPF-HJDGSVD outperforms CPF-JDGSVD considerably in terms of outer iterations and overall efficiency, and IF-HJDGSVD is slightly better than CPF-HJDGSVD as it uses quite fewer outer iterations and slightly fewer inner iterations and less CPU time than the latter one. Clearly, both CPF-HJDGSVD and IF-HJDGSVD are suitable for this problem and IF-HJDGSVD is favorable due to the faster outer convergence.

In summary, for the four test problems, IF-HJDGSVD performs best, CPF-HJDGSVD is the second, and both of them are considerably better than CPF-JDGSVD.

Example 5.4. We compute the ten GSVD components of $(A, B) = (grid2, L_1)$ with the desired generalized singular values closest to the target $\tau = 4e + 2$. The desired generalized singular values are the largest ones and well separated one another.

For the matrix pairs (A,B) with B rank deficient, CPF-HJDGSVD cannot be applied. We only use CPF-JDGSVD and IF-HJDGSVD to compute the desired GSVD components of (A,B) and report the results obtained. The outer iterations, inner iterations and CPU time used by CPF-JDGSVD are 48, 71317 and 6.6 seconds, respectively, and those used by IF-HJDGSVD are 42, 67463 and 6.3 seconds, respectively. In Figure 5, we draw the outer convergence curves of these two algorithms.

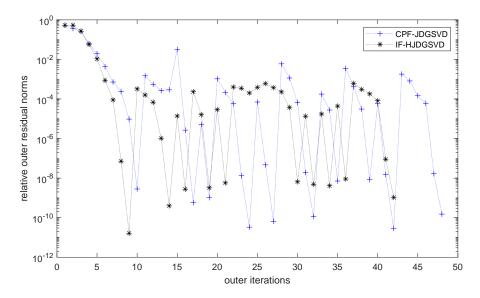


Fig. 5. Computing ten GSVD components of $(A, B) = (grid2, L_1)$ with $\tau = 4e + 2$.

As can be seen from Figure 5 and the data listed above, IF-HJDGSVD outperforms CPF-JDGSVD in terms of the outer iterations, the overall efficiency and smoother convergence behavior.

Example 5.5. We compute the ten GSVD components of the matrix pairs $(A_1, B_1) = (dw1024, L_1), (A_2, B_2) = (r05^T, L_1), (A_3, B_3) = (p05^T, L_1), (A_4, B_4) = (bibd_81_2, L_2), (A_5, B_5) = (benzene, L_2) and <math>(A_6, B_6) = (blckhole, L_2)$ with the generalized singular values closest to the targets $\tau_1 = 30, \tau_2 = 40, \tau_3 = 300, \tau_4 = 150, \tau_5 = 3$ and $\tau_6 = 400$, respectively. All the desired generalized singular values are interior ones and are fairly clustered, except for (A_1, B_1) , whose desired generalized singular values are well separated one another.

Table 3
Results on test matrix pairs in Example 5.5

A	(CPF-JDGS	VD	IF-HJDGSVD			
	I_{out}	I_{in}	T_{cpu}	I_{out}	I_{in}	T_{cpu}	
dw1024	62	61063	3.61	47	49560	2.86	
$r05^T$	73	58292	14.9	44	56257	15.0	
$p05^T$	48	111177	24.7	40	96114	22.5	
$bibd_81_2$	166	484601	39.9	112	314748	27.3	
benzene	65	154109	88.9	41	109394	61.3	
blckhole	180	356204	23.5	128	242227	16.1	

Table 3 displays all the results obtained. As is observed from them, for the matrix pairs (A_1, B_1) , (A_3, B_3) , (A_4, B_4) , (A_5, B_5) and (A_6, B_6) with the given targets, IF-HJDGSVD uses fewer outer and inner iterations and less CPU time to converge than CPF-JDGSVD, and it outperforms CPF-JDGSVD either slightly or significantly. For (A_2, B_2) , however, IF-HJDGSVD uses much fewer outer iterations but comparable inner iterations and CPU time to compute all the desired GSVD components,

compared with CPF-JDGSVD. In terms of a smoother and faster outer convergence, IF-HJDGSVD outperforms CPF-JDGSVD for this problem; almost the same overall efficiency, i.e., I_{inner} and T_{cpu} , is due to approximate solutions of correction equations using the MINRES method, whose convergence is complicated and depends on several factors, especially when a linear system is highly indefinite.

Summarizing all the numerical experiments, we conclude that (i) for the computation of large GSVD components, CPF-HJDGSVD and IF-HJDGSVD generally suit better than CPF-JDGSVD, (ii) for the computation of interior GSVD components, CPF-HJDGSVD and IF-HJDGSVD generally outperform CPF-JDGSVD, and, of them, IF-HJDGSVD is often favorable due to its faster and smoother convergence, higher overall efficiency and wider applicability, and (iii) for the computation of small GSVD components, if B is of full column rank, then CPF-HJDGSVD performs slightly better than IF-HJDGSVD and both of them are preferable to CPF-JDGSVD.

6. Conclusions. In this paper, we have proposed two harmonic extraction based JDGSVD methods CPF-HJDGSVD and IF-HJDGSVD that are more suitable for the computation of interior GSVD components of a large matrix pair. The algorithms are A^TA and B^TB free and their inversions free, respectively. To be practical, we have developed their thick-restart algorithms with efficient deflation and purgation to compute more than one GSVD components of (A, B) with a given target τ . We have detailed a number of key issues on subtle efficient implementations.

We have made numerical experiments on a number of problems, illustrating that both IF-HJDGSVD and CPF-HJDGSVD outperform CPF-JDGSVD and can be much better than CPF-JDGSVD, especially for the computation of interior GSVD components. Furthermore, we have observed that IF-HJDGSVD is generally more robust and reliable than CPF-HJDGSVD and, therefore, is preferable but CPF-HJDGSVD is a better option when small GSVD components are required and B has full column rank.

However, as we have observed, IF-HJDGSVD and CPF-HJDGSVD, though better than CPF-JDGSVD, may perform badly for some test problems, and they may exhibit irregular convergence behavior. This is most probably due to the intrinsic possible irregular convergence and even non-convergence of a harmonic extraction approach, which states that harmonic Ritz vectors may converge irregularly and even fail to converge even though the distances between desired eigenvectors or, equivalently, (generalized) singular vectors and searching subspaces tend to zero; see [19]. Such potential drawback has severe effects on effective expansions of searching subspaces and strongly affects the convergence of the resulting harmonic extraction based algorithms. To better solve the GSVD problem in this paper, a refined or refined harmonic extraction based JDGSVD type algorithm should be appealing. This will constitute our future work.

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