Asymptotic Quadratic Convergence of the Two-Sided Serial and Parallel Block-Jacobi SVD Algorithm

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Abstract. *This report is devoted to the proof of the global convergence and asymptotic quadratic convergence of the serial and parallel two-sided block-Jacobi SVD algorithm. In the serial case, one pair of the off-diagonal blocks with the largest weight given as the sum of squares of Frobenius norms is annihilated. In the parallel case, using the greedy implementation of dynamic ordering and having p processors, p pairs of the off-diagonal blocks with largest weights and disjunct block row and column indices are annihilated in each parallel iteration step.*

1 Serial two-sided SVD algorithm

It is assumed in this report that the singular value decomposition is computed for a square matrix. Hence, when the original matrix is of size $m \times n$, $m \geq n$, compute first its QR decomposition and then apply the SVD algorithm to the $n \times n$ factor R.

Let us divide a square matrix A of order n into a $w \times w$ block structure with w blocks in each block row (column). Denote by A_{IJ} the (I, J)th block of size $\ell \times \ell$, $\ell = n/w$. Hence, there are $w(w-1)$ off-diagonal blocks in A.

Let us assume that, at the initialization step, all diagonal blocks of A were diagonalized by a series of unitary, two-sided transformations. Diagonal blocks remain then diagonal during the whole computation.

In the kth step of the two-sided serial block-Jacobi SVD method, let us define weights for

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off-diagonal blocks with symmetric block indices (I, J) and (J, I), $I \neq J$, by

$$w_{IJ}^{(k)} \equiv \|A_{IJ}^{(k)}\|_F^2 + \|A_{JI}^{(k)}\|_F^2. \tag{1}$$

To optimally reduce the off-diagonal Frobenius norm, the pair of off-diagonal blocks with the *maximal* weight will be eliminated. Let these off-diagonal blocks have block indices (X_k, Y_k) and (Y_k, X_k), i.e.

$$w_{X_kY_k}^{(k)} = \max_{I \neq J} w_{IJ}^{(k)}.$$

Notice that, contrary to the EVD of Hermitian matrices, choosing two off-diagonal blocks with maximal weight for annihilation is *not* equivalent to choosing the off-diagonal block $A_{S_kT_k}^{(k)}$ with the *largest* Frobenius norm together with the block $A_{T_kS_k}^{(k)}$. In fact, one can easily have

$$w_{S_kT_k}^{(k)} < w_{X_kY_k}^{(k)},$$

so that the off-diagonal block with the largest Frobenius norm is not eliminated.

The annihilation is performed by a two-sided unitary transformation

$$(U^{(k)})^H A^{(k)} V^{(k)} = A^{(k+1)},$$

where the $n \times n$ unitary matrices $U^{(k)}$ and $V^{(k)}$ are the matrices of local left and right singular vectors, respectively, embedded into the identity matrix I_n of size n. Four blocks of $U^{(k)}$ and $V^{(k)}$, each of size ℓ, that are different from blocks of I_n can be chosen so that

$$\begin{pmatrix} U_{X_kX_k}^{(k)} & U_{X_kY_k}^{(k)} \\ U_{Y_kX_k}^{(k)} & U_{Y_kY_k}^{(k)} \end{pmatrix}^H \begin{pmatrix} A_{X_kX_k}^{(k)} & A_{X_kY_k}^{(k)} \\ A_{Y_kX_k}^{(k)} & A_{Y_kY_k}^{(k)} \end{pmatrix} \begin{pmatrix} V_{X_kX_k}^{(k)} & V_{X_kY_k}^{(k)} \\ V_{Y_kX_k}^{(k)} & V_{Y_kY_k}^{(k)} \end{pmatrix} = \begin{pmatrix} A_{X_kX_k}^{(k+1)} & 0 \\ 0 & A_{Y_kY_k}^{(k+1)} \end{pmatrix}, \tag{2}$$

whereby the diagonal blocks $A_{X_kX_k}^{(k+1)}$ and $A_{Y_kY_k}^{(k+1)}$ are square, diagonal matrices of order ℓ with non-negative diagonal elements (local singular values).

Let us define

$$\tilde{U}^{(k)} \equiv \begin{pmatrix} U_{X_kX_k}^{(k)} & U_{X_kY_k}^{(k)} \\ U_{Y_kX_k}^{(k)} & U_{Y_kY_k}^{(k)} \end{pmatrix}, \quad \tilde{V}^{(k)} \equiv \begin{pmatrix} V_{X_kX_k}^{(k)} & V_{X_kY_k}^{(k)} \\ V_{Y_kX_k}^{(k)} & V_{Y_kY_k}^{(k)} \end{pmatrix}, \tag{3}$$

and

$$\tilde{A}^{(k)} \equiv \begin{pmatrix} A_{X_kX_k}^{(k)} & A_{X_kY_k}^{(k)} \\ A_{Y_kX_k}^{(k)} & A_{Y_kY_k}^{(k)} \end{pmatrix}, \quad \Sigma^{(k)} \equiv \begin{pmatrix} A_{X_kX_k}^{(k+1)} & 0 \\ 0 & A_{Y_kY_k}^{(k+1)} \end{pmatrix}. \tag{4}$$

Since Eq. (2) is essentially the SVD of the matrix $\tilde{A}^{(k)}$, the matrix $\tilde{U}^{(k)}$ and $\tilde{V}^{(k)}$ is the unitary matrix of left and right singular vectors of $\tilde{A}^{(k)}$, respectively.

To prove the global convergence of the parallel two-sided block-Jacobi SVD method, let us define the square of the off-diagonal Frobenius norm of $A^{(k)}$ by

$$\|\mathrm{off}(A^{(k)})\|_F^2 \equiv \sum_{I \neq J} \|A_{IJ}^{(k)}\|_F^2. \tag{5}$$

Then:

$$\begin{aligned} \|\mathrm{off}(A^{(k+1)})\|_F^2 &= \|\mathrm{off}(A^{(k)})\|_F^2 - (\|A^{(k)}_{X_kY_k}\|_F^2 + \|A^{(k)}_{Y_kX_k}\|_F^2) \\ &\le \left(1 - \frac{2}{w(w-1)}\right) \|\mathrm{off}(A^{(k)})\|_F^2. \end{aligned}$$

Here we used the bound

$$\|\mathrm{off}(A^{(k)})\|_F^2 \le \frac{w(w-1)}{2}(\|A^{(k)}_{X_kY_k}\|_F^2 + \|A^{(k)}_{Y_kX_k}\|_F^2).$$

Hence, $\|\mathrm{off}(A^{(k)})\|_F^2$ decreases at least as fast as the geometric sequence with the quotient $(W-1)/W$, $W = w(w-1)/2$, and therefore converges to zero. Note that this proof does not depend on the distribution of singular values of A.

The singular values of $\tilde{A}^{(k)}$, i.e., the diagonal elements of the diagonal matrix $\hat{A}^{(k+1)}$, can be computed and located on the diagonal in any order. An important variant of the local SVD is that with *ordered* singular values (e.g., non-increasingly) on the diagonal of $\hat{A}^{(k+1)}$. This can be achieved in $O(\ell^2)$ steps using a suitable permutation matrix $\Pi^{(k)}$:

$$\begin{aligned} \tilde{A}^{(k)} &= \tilde{U}^{(k)} \hat{A}^{(k+1)} (\tilde{V}^{(k)})^H \\ &= \left(\tilde{U}^{(k)} (\Pi^{(k)})^H\right) \left(\Pi^{(k)} \hat{A}^{(k+1)} (\Pi^{(k)})^H\right) \left(\tilde{V}^{(k)} (\Pi^{(k)})^H\right)^H. \end{aligned}$$

This variant of the SVD of a 2×2 block subproblem will be called the *local ordering of diagonal elements (LODE).*

1.1 Asymptotic quadratic convergence

Using these preliminaries, we investigate the asymptotic convergence property of the serial two-sided block-Jacobi SVD method in a general setting when no *a priori* assumptions about the distribution of singular values of A are made.

In the following, we sometimes drop the superscript (k) when there is no reason for misunderstanding. In that case, we use quantities with hat (like $\hat{A}$) to denote them at the $(k+1)$th step.

First lemma is an obvious modification of Lemma 1 in [6]. It is devoted to the change of the Frobenius norm of a non-eliminated off-diagonal block in a given iteration step. Notice that one iteration step changes only two block rows and two block columns X, Y. The lemma considers the block row and block column X. The situation for the block row and column Y is similar.

Lemma 1 *Let A_{ST} be the off-diagonal block with the largest Frobenius norm. Consider the change of an off-diagonal block A_{XJ} ($J \neq X, Y$) after elimination of A_{XY}:*

$$\hat{A}_{XJ} = U_{XX}^H A_{XJ} + U_{YX}^H A_{YJ}. \tag{6}$$

Similarly, consider the change of an off-diagonal block A_{JX} ($J \neq X, Y$) after elimination of A_{YX}:

$$\hat{A}_{JX} = A_{JX} V_{XX} + A_{JY} V_{YX}. \tag{7}$$

Let $C = (A_{XY}, A_{YX})$. *If* $\begin{pmatrix} U_{YX} \\ V_{YX} \end{pmatrix}$ *of size* $2\ell \times \ell$ *is bounded as* $\left\| \begin{pmatrix} U_{YX} \\ V_{YX} \end{pmatrix} \right\|_2 \leq \|C\|_F/\delta$ *for some constant* $\delta > 0$*, then the following inequalities hold:*

$$\left| \|\hat{A}_{XJ}\|_F^2 - \|A_{XJ}\|_F^2 \right| \leq \frac{\|A_{ST}\|_F^2}{\delta^2} \|C\|_F^2 + 2\frac{\|A_{ST}\|_F}{\delta} \|C\|_F \|A_{XJ}\|_F, \tag{8}$$

$$\left| \|\hat{A}_{JX}\|_F^2 - \|A_{JX}\|_F^2 \right| \leq \frac{\|A_{ST}\|_F^2}{\delta^2} \|C\|_F^2 + 2\frac{\|A_{ST}\|_F}{\delta} \|C\|_F \|A_{JX}\|_F. \tag{9}$$

Proof: Since

$$\max\{\|U_{YX}\|_2, \|V_{YX}\|_2\} \leq \left\| \begin{pmatrix} U_{YX} \\ V_{YX} \end{pmatrix} \right\|_2 \leq \frac{\|C\|_F}{\delta},$$

and both transformations in Eqs. (6) and (7) are one-sided by corresponding blocks of 2×2 block unitary matrices of local left and right singular vectors, respectively, the changes of Frobenius norms can be bounded using the same technique as in the proof of Lemma 1 of [6]:

$$\begin{aligned} &\left| \|\hat{A}_{XJ}\|_F^2 - \|A_{XJ}\|_F^2 \right| \\ &\leq \|U_{YX}\|_2^2 \max\left\{ \|A_{XJ}\|_F^2, \|A_{YJ}\|_F^2 \right\} + 2\|A_{XJ}\|_F \|U_{YX}\|_2 \|A_{YJ}\|_F \\ &\leq \frac{\|A_{ST}\|_F^2}{\delta^2} \|C\|_F^2 + 2\,\frac{\|A_{ST}\|_F}{\delta} \|C\|_F \|A_{XJ}\|_F. \end{aligned}$$

Similar approach is valid also for Eq. (9). □

Next theorem contains our main result—the proof of the asymptotic quadratic convergence after $W = w(w-1)/2$ steps of the serial two-sided block-Jacobi SVD algorithm. Its proof is almost identical to the proof of Theorem 1 in [6] and only minor adjustments are needed.

Theorem 1 *Consider one sweep* ($W = w(w-1)/2$ *eliminations) of the block-Jacobi method. Without loss of generality, denote the iteration steps by* $k = 0, 1, \ldots, W-1$ *and the off-diagonal blocks chosen at step* k *for annihilation as* $A^{(k)}_{X_kY_k}$ *and* $A^{(k)}_{Y_kX_k}$*. Let* $C^{(k)} = (A^{(k)}_{X_kY_k}, A^{(k)}_{Y_kX_k})$*, and let* $A^{(k)}_{S_kT_k}$ *be the off-diagonal block with the maximal Frobenius norm at iteration step* k*. If all matrices* $\begin{pmatrix} U^{(k)}_{Y_kX_k} \\ V^{(k)}_{Y_kX_k} \end{pmatrix}$ *used at iteration steps* $k = 0, 1, \ldots, W-1$ *satisfy* $\left\| \begin{pmatrix} U^{(k)}_{Y_kX_k} \\ V^{(k)}_{Y_kX_k} \end{pmatrix} \right\|_2 \leq \|C^{(k)}\|_F/\delta$ *for some constant* $\delta > 0$*, then*

$$\|\text{off}(A^{(W)})\|_F^2 \leq \frac{w-2}{2} \left(\frac{2\|\text{off}(A^{(0)})\|_F^2}{\delta} \right)^2, \tag{10}$$

i.e., the block-Jacobi SVD algorithm converges quadratically after every sweep W*.*

Proof: We show that for each $k = 0, 1, \ldots, W$, there exists a symmetric index set $\mathcal{P}_k = \{(I,J),(J,I) | I \neq J\}$ such that $|\mathcal{P}_k| = 2k$ and

$$\sum_{(I,J)\in\mathcal{P}_k} \|A^{(k)}_{IJ}\|_F^2 \leq \frac{w-2}{2} \left(\frac{2\|\text{off}(A^{(0)})\|_F^2 - 2\|\text{off}(A^{(k)})\|_F^2}{\delta} \right)^2. \tag{11}$$

Note that when $k = W$, the left-hand side becomes $\|\mathrm{off}(A^{(W)})\|_F^2$, and the right-hand side is smaller than the right-hand side of Eq. (10). So it is sufficient to prove Eq. (11) instead of Eq. (10). Eq. (11) will be proved by induction. When $k = 0$, it holds trivially because both sides are zero. We assume that Eq. (11) holds for some k $(0 \leq k < W)$ and show that it also holds for $k + 1$.

Let us choose the $2k$ off-diagonal blocks of $A^{(k)}$ that give k smallest weights, which are computed according to Eq. (1). Denote their index set by $\mathcal{P}'_k$. It follows from the definition of weights that the set $\mathcal{P}'_k$ is symmetric, i.e., if $(I, J) \in \mathcal{P}'_k$ then $(J, I) \in \mathcal{P}'_k$, and $(X_k, Y_k) \notin \mathcal{P}'_k$. Notice that Eq. (11) holds also for $\mathcal{P}'_k$. Now, let $\mathcal{P}_{k+1} = \mathcal{P}'_k \cup \{(X_k, Y_k), (Y_k, X_k)\}$. Then $\mathcal{P}_{k+1}$ is symmetric, $|\mathcal{P}_{k+1}| = 2(k + 1)$ and the left-hand side of Eq. (11) for $k + 1$ can be computed as

$$
\begin{aligned}
\sum_{(I,J)\in\mathcal{P}_{k+1}} \|A_{IJ}^{(k+1)}\|_F^2 &= \sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k+1)}\|_F^2 + \|A_{X_kY_k}^{(k+1)}\|_F^2 + \|A_{Y_kX_k}^{(k+1)}\|_F^2 \\
&\leq \sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k)}\|_F^2 + \sum_{(I,J)\in\mathcal{Q}_k} \left| \|A_{IJ}^{(k+1)}\|_F^2 - \|A_{IJ}^{(k)}\|_F^2 \right|,
\end{aligned} \tag{12}
$$

where the symmetric index set $\mathcal{Q}_k \subseteq \mathcal{P}'_k$ is defined as

$$
\begin{aligned}
\mathcal{Q}_k \equiv &\{(X_k, J), (J, X_k) | (X_k, J) \in \mathcal{P}'_k, (Y_k, J) \notin \mathcal{P}'_k\} \\
&\cup \{(Y_k, J), (J, Y_k) | (Y_k, J) \in \mathcal{P}'_k, (X_k, J) \notin \mathcal{P}'_k\}.
\end{aligned}
$$

To derive the second inequality in Eq. (12), we used the fact that both $A_{X_kY_k}^{(k+1)}$ and $A_{Y_kX_k}^{(k+1)}$ become zero due to elimination. We also used the fact that when $(I, J) \in \mathcal{P}'_k \backslash \mathcal{Q}_k$, either $A_{IJ}^{(k)}$ is not affected by the elimination, or both (X_k, J) and (Y_k, J) (or (J, X_k) and (J, Y_k)) belong to $\mathcal{P}'_k$ and therefore the sum of squares of the Frobenius norms of these two blocks is not changed after elimination. Hence, the change of $A_{IJ}^{(k)}$ contributes to the change of $\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k)}\|_F^2$ only when $(I, J) \in \mathcal{Q}_k$.

Now we evaluate the second term of Eq. (12). Let us consider the case of $I = X_k$ and $J \neq X_k, Y_k$. From the assumption $\|U_{Y_kX_k}^{(k)}\|_2 \leq \|C^{(k)}\|_F/\delta$ and Lemma 1,

$$
\left| \|A_{X_kJ}^{(k+1)}\|_F^2 - \|A_{X_kJ}^{(k)}\|_F^2 \right| \leq \frac{\|A_{S_kT_k}^{(k)}\|_F^2}{\delta^2} \|C^{(k)}\|_F^2 + 2\frac{\|A_{S_kT_k}^{(k)}\|_F}{\delta} \|C^{(k)}\|_F \|A_{X_kJ}^{(k)}\|_F. \tag{13}
$$

Other cases can be treated in similar way (using also $\|V_{Y_kX_k}^{(k)}\|_2 \leq \|C^{(k)}\|_F/\delta$). Noting that $|\mathcal{Q}_k| < 2w - 4$ (since only one of (X_k, J) and (Y_k, J) (or (J, X_k) and (J, Y_k)) can belong to $\mathcal{Q}_k$), we have

$$
\begin{aligned}
\sum_{(I,J)\in\mathcal{Q}_k} \|A_{IJ}^{(k)}\|_F &\leq \sqrt{2w - 4} \sqrt{\sum_{(I,J)\in\mathcal{Q}_k} \|A_{IJ}^{(k)}\|_F^2} \\
&\leq \sqrt{2w - 4} \sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k)}\|_F^2},
\end{aligned} \tag{14}
$$

where we used the Cauchy-Schwarz inequality in the first inequality and $\mathcal{Q}_k \subseteq \mathcal{P}'_k$ in the second inequality. By combining Eqs. (13) and (14), we can evaluate the second term of Eq. (12) as

$$\sum_{(I,J)\in\mathcal{Q}_k} \left| \|A_{IJ}^{(k+1)}\|_F^2 - \|A_{IJ}^{(k)}\|_F^2 \right| \le \frac{(2w-4)\,\|A_{S_kT_k}^{(k)}\|_F^2 \|C^{(k)}\|_F^2}{\delta^2} +$$
$$+ \frac{2\sqrt{2w-4}\,\|A_{S_kT_k}^{(k)}\|_F \|C^{(k)}\|_F}{\delta} \sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k)}\|_F^2}.$$

Inserting this upper bound into Eq. (12), and using the estimate

$$\|A_{S_kT_k}^{(k)}\|_F \le \sqrt{\|A_{X_kY_k}^{(k)}\|_F^2 + \|A_{Y_kX_k}^{(k)}\|_F^2} = \|C^{(k)}\|_F$$

one finally gets:

$$\begin{aligned}
\sum_{(I,J)\in\mathcal{P}_{k+1}} \|A_{IJ}^{(k+1)}\|_F^2 \;&\le\; \left(\frac{\sqrt{2w-4}\,\|C^{(k)}\|_F^2}{\delta} + \sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k)}\|_F^2} \right)^2 \\
&\le\; \left(\frac{\sqrt{2w-4}\,\|C^{(k)}\|_F^2}{\delta} + \frac{\sqrt{2w-4}\,(2\|\mathrm{off}(A^{(0)})\|_F^2 - 2\|\mathrm{off}(A^{(k)})\|_F^2)}{2\delta} \right)^2 \\
&=\; \frac{w-2}{2} \left(\frac{2\|\mathrm{off}(A^{(0)})\|_F^2 - 2\|\mathrm{off}(A^{(k+1)})\|_F^2}{\delta} \right)^2 .
\end{aligned}$$

Here we used Eq. (11) in the second inequality, which is valid also for $\mathcal{P}'_k$ since by its construction:

$$\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k)}\|_F^2 \le \sum_{(I,J)\in\mathcal{P}_k} \|A_{IJ}^{(k)}\|_F^2.$$

The last equality comes from

$$2\|\mathrm{off}(A^{(k+1)})\|_F^2 = 2\|\mathrm{off}(A^{(k)})\|_F^2 - 2\|C^{(k)}\|_F^2.$$

The final upper bound shows that Eq. (11) holds also for $k+1$ and this completes the proof.□

1.2 Well-separated singular values

Now we identify the constant δ for well-separated singular values. Let A be a square matrix of order n with q different singular values:

$$\sigma_1 = \cdots = \sigma_{s_1} > \sigma_{s_1+1} = \cdots = \sigma_{s_2} > \cdots > \sigma_{s_{q-1}+1} = \cdots = \sigma_{s_q},$$

where $n_i = s_i - s_{i-1}$, $1 \le i \le q$, is the multiplicity of σ_{s_i} (defining $s_0 = 0$ and $s_q = n$). Let the *gap* d be defined as

$$d \equiv \min_{i\neq j} |\sigma_{s_i} - \sigma_{s_j}|. \tag{15}$$

Writing

$$A^{(k)} = \mathrm{diag}(A^{(k)}) + \mathrm{off}(A^{(k)}), \tag{16}$$

we can make following assumptions at some iteration step k:

A1 The off-diagonal Frobenius norm of $A^{(k)}$ is small enough:

$$\|\text{off}(A^{(k)})\|_F \equiv \sqrt{\sum_{I\neq J} \|A_{IJ}^{(k)}\|_F^2} < \frac{d}{4}. \tag{17}$$

A2 The main diagonal of $A^{(k)}$ is ordered (e.g., non-increasingly) by suitable row and column permutations so that the diagonal elements of $A^{(k)}$ affiliated with the same multiple singular value occupy successive positions on the diagonal.

A3 The partition of $A^{(k)}$ is such that the diagonal elements affiliated with the same multiple singular value are confined to one diagonal block. □

When $d = 0$, Eq. (17) gives $\|\text{off}(A^{(k)})\|_F = 0$ and, consequently, $A^{(k)} = \sigma_1 I$, so that the matrix is already diagonal. Therefore we assume $q > 1$.

Since all transformations are unitary, the singular values of A are the same as those of $A^{(k)}$. But then, according to Eq. (16), $\text{off}(A^{(k)})$ is a perturbation of $\text{diag}(A^{(k)})$, and it is bounded in the Frobenius norm by $d/4$ because of **A1**. According to the Hoffman-Wielandt theorem [5, 7], which is valid also for singular values, for each i, $1 \leq i \leq q$, there are exactly n_i diagonal elements of $A^{(k)}$ that lie around σ_{s_i} in the circle of radius less than $d/4$. Recall that according to the assumption **A2** these diagonal elements occupy successive positions on the diagonal, i.e. they form *clusters* $\widehat{Cl}_i^{(k)}$, $1 \leq i \leq q$. Note that, at iteration step k, two different clusters are separated *at least* by $d/2$.

Now we show that these clusters are *stabilized*, i.e., a diagonal element that lies in the circle around σ_{s_i} can not 'jump' into a circle around σ_{s_j} for $j \neq i$.

Lemma 2 *Under assumptions* **A1**–**A3***, let a cluster* $\widehat{Cl}_i^{(k)}$*,* $1 \leq i \leq q$*, lie inside the diagonal block* $A_{tt}^{(k)}$ *for some fixed* t*,* $1 \leq t \leq w$*. Assume that the algorithm uses the LODE in each iteration step. Then, for all iteration steps* r*,* $r \geq k$*,* n_i *elements of* $\widehat{Cl}_i^{(r)}$ *occupy successive positions on the diagonal inside the same diagonal block* $A_{tt}^{(r)}$*. Consequently, the distance between any two different clusters remains at least* $d/2$*.*

Proof: The proof is identical to that of Lemma 2 in [6]. □

The stabilization of clusters of diagonal elements means that the diagonal elements of $\tilde{A}^{(r)}$ and $\hat{A}^{(r+1)}$ approximate the *same* singular values of A with the *same* number of corresponding diagonal elements for $r \geq k$. Moreover, due to the LODE, the diagonal elements of both $\tilde{A}^{(r)}$ and $\hat{A}^{(r+1)}$ are ordered in the same way, e.g. non-increasingly.

Finally, next lemma gives the value of constant δ.

Lemma 3 *In the case of well-separated singular values (simple and/or multiple) of* A*, under assumptions* **A1**–**A3** *above and using the LODE, the constant* δ *in Theorem 1 can be set to* $\delta = \sqrt{2}d/4$ *where* d *is the gap defined by Eq. (15).*

Proof: Let us analyze one iteration step $r \to r+1$, $r \geq k$. Recall that the 2×2 block subproblem from Eq. (2) has the form:

$$\begin{pmatrix} A_{XX}^{(r)} & A_{XY}^{(r)} \\ A_{YX}^{(r)} & A_{YY}^{(r)} \end{pmatrix} \begin{pmatrix} V_{XX}^{(r)} & V_{XY}^{(r)} \\ V_{YX}^{(r)} & V_{YY}^{(r)} \end{pmatrix} = \begin{pmatrix} U_{XX}^{(r)} & U_{XY}^{(r)} \\ U_{YX}^{(r)} & U_{YY}^{(r)} \end{pmatrix} \begin{pmatrix} A_{XX}^{(r+1)} & 0 \\ 0 & A_{YY}^{(r+1)} \end{pmatrix}.$$

Applying the Hermitian operator, using the fact that both $\tilde{U}^{(r)}$ and $\tilde{V}^{(r)}$ are unitary (see Eq. (3)), and noting that the diagonal blocks $A_{XX}^{(r)}, A_{YY}^{(r)}$, $A_{XX}^{(r+1)}$ and $A_{YY}^{(r+1)}$ are diagonal and real, one gets the additional relation

$$\begin{pmatrix} A_{XX}^{(r)} & A_{YX}^{(r)H} \\ A_{XY}^{(r)H} & A_{YY}^{(r)} \end{pmatrix} \begin{pmatrix} U_{XX}^{(r)} & U_{XY}^{(r)} \\ U_{YX}^{(r)} & U_{YY}^{(r)} \end{pmatrix} = \begin{pmatrix} V_{XX}^{(r)} & V_{XY}^{(r)} \\ V_{YX}^{(r)} & V_{YY}^{(r)} \end{pmatrix} \begin{pmatrix} A_{XX}^{(r+1)} & 0 \\ 0 & A_{YY}^{(r+1)} \end{pmatrix}.$$

Now take the equations for the block $(2,1)$ from both relations:

$$\begin{aligned} A_{YY}^{(r)} V_{YX}^{(r)} - U_{YX}^{(r)} A_{XX}^{(r+1)} &= -A_{YX}^{(r)} V_{XX}^{(r)}, \\ A_{YY}^{(r)} U_{YX}^{(r)} - V_{YX}^{(r)} A_{XX}^{(r+1)} &= -A_{XY}^{(r)H} U_{XX}^{(r)}. \end{aligned}$$

This system can be written as the Sylvester equation [3] for $\begin{pmatrix} U_{YX}^{(r)} \\ V_{YX}^{(r)} \end{pmatrix}$:

$$\begin{pmatrix} 0 & A_{YY}^{(r)} \\ A_{YY}^{(r)} & 0 \end{pmatrix} \begin{pmatrix} U_{YX}^{(r)} \\ V_{YX}^{(r)} \end{pmatrix} - \begin{pmatrix} U_{YX}^{(r)} \\ V_{YX}^{(r)} \end{pmatrix} A_{XX}^{(r+1)} = -\begin{pmatrix} A_{YX}^{(r)} V_{XX}^{(r)} \\ A_{XY}^{(r)H} U_{XX}^{(r)} \end{pmatrix}. \tag{18}$$

Notice that the blocks $A_{YY}^{(r)}$ and $A_{XX}^{(r+1)}$ are diagonal and their eigenvalues are diagonal elements, which are all non-negative. Hence, the spectrum of the first matrix on the left-hand side of Eq. (18), denoted by $E^{(r)} = \begin{pmatrix} 0 & A_{YY}^{(r)} \\ A_{YY}^{(r)} & 0 \end{pmatrix}$, consists of diagonal elements of $A_{YY}^{(r)}$, whereby each diagonal element is present with the plus and minus sign. Recall that according to the construction of matrix partition, the eigenvalues of $A_{YY}^{(r)}$ and $A_{XX}^{(r+1)}$ approximate *different* singular values of A. Using Lemma 2, the spectra of $E^{(r)}$ and $A_{XX}^{(r+1)}$ are disjoint, and the entire spectrum of $A_{XX}^{(r+1)}$ lies, on the real axis, either to the right of the entire spectrum of $E^{(r)}$, or between its positive and negative part. Thus the distance between the spectra of $E^{(r)}$ and $A_{XX}^{(r+1)}$ is at least $d/2$. Therefore, we can apply the Davis-Kahan lemma [1] stating that the Sylvester equation (18) has the unique solution $\begin{pmatrix} U_{YX}^{(r)} \\ V_{YX}^{(r)} \end{pmatrix}$ and its spectral norm is bounded by

$$\begin{aligned} \left\| \begin{pmatrix} U_{YX}^{(r)} \\ V_{YX}^{(r)} \end{pmatrix} \right\|_2 &\leq \frac{2}{d} \left\| -\begin{pmatrix} A_{YX}^{(r)} V_{XX}^{(r)} \\ A_{XY}^{(r)H} U_{XX}^{(r)} \end{pmatrix} \right\|_2 = \frac{2}{d} \left\| \begin{pmatrix} A_{YX}^{(r)} & 0 \\ 0 & A_{XY}^{(r)H} \end{pmatrix} \begin{pmatrix} V_{XX}^{(r)} \\ U_{XX}^{(r)} \end{pmatrix} \right\|_2 \\ &\leq \frac{2}{d} \left\| \begin{pmatrix} A_{YX}^{(r)} & 0 \\ 0 & A_{XY}^{(r)H} \end{pmatrix} \right\|_F \left\| \begin{pmatrix} V_{XX}^{(r)} \\ U_{XX}^{(r)} \end{pmatrix} \right\|_2 \\ &= \frac{2}{d} \|C^{(r)}\|_F \left\| \begin{pmatrix} V_{XX}^{(r)} \\ U_{XX}^{(r)} \end{pmatrix} \right\|_2 . \end{aligned}$$

However,

$$\begin{aligned}\left\| \begin{pmatrix} V_{XX}^{(r)} \\ U_{XX}^{(r)} \end{pmatrix} \right\|_2^2 &= \left\| (V_{XX}^{(r)H} U_{XX}^{(r)H}) \begin{pmatrix} V_{XX}^{(r)} \\ U_{XX}^{(r)} \end{pmatrix} \right\|_2 = \|V_{XX}^{(r)H} V_{XX}^{(r)} + U_{XX}^{(r)H} U_{XX}^{(r)}\|_2 \\ &\leq \|V_{XX}^{(r)H} V_{XX}^{(r)}\|_2 + \|U_{XX}^{(r)H} U_{XX}^{(r)}\|_2 \leq 2,\end{aligned}$$

so that

$$\left\| \begin{pmatrix} U_{YX}^{(r)} \\ V_{YX}^{(r)} \end{pmatrix} \right\|_2 \leq \frac{2\sqrt{2}}{d} \|C^{(r)}\|_F.$$

Hence, $\delta = \sqrt{2}d/4$ and the asymptotic quadratic convergence proved in Theorem 1 is ensured. □

1.3 Clusters of singular values

If A has singular values that can be divided into one or more tight clusters, the quantity d in Eq. (15) can be tiny. Then the assumption **A1** in subsection 1.2 becomes useless in practice because it requires that $\|\mathrm{off}(A^{(k)})\|_F$ is even smaller than d. For such a situation, Hari [4] suggested to use another spectral gap d_c which can be much larger than d.

Let us group the singular values of A into q sets of very close ones (clusters):

$$Cl_i = \{\sigma_{s_{i-1}+1}, \ldots, \sigma_{s_i}\}, \quad 1 \leq i \leq q,$$

where $s_0 = 0,\ s_q = n$. As above, $n_i = s_i - s_{i-1} \geq 1$ is the number of eigenvalues inside the ith cluster Cl_i. For each cluster, define its average value,

$$c_i \equiv \frac{1}{n_i} \sum_{j=1}^{n_i} \sigma_{s_{i-1}+j}$$

and assume that c_i's are ordered decreasingly, $c_1 > c_2 > \ldots > c_q$.

Let $A = U\Sigma V^H$ be the SVD of A and write

$$\Sigma = \Sigma_c + \Sigma_E, \quad \text{where} \quad \Sigma_c = \mathrm{diag}(c_1, \ldots, c_1, \ldots, c_q, \ldots, c_q)$$

with c_i, $1 \leq i \leq q$, repeated n_i times. Then

$$A = A_c + E, \quad A_c = U\Sigma_c V^H, \quad E = U\Sigma_E V^H.$$

A_c has multiple singular values c_i, $1 \leq i \leq q$, and $\|E\|_F$ is tiny for tight clusters. In particular, $\|E\|_2$ is the half-width of the largest cluster and (see [4])

$$\|E\|_F = \sqrt{\sum_{i=1}^{q} \sum_{j=1}^{n_i} |\sigma_{s_{i-1}+j} - c_i|^2}.$$

As in [4], let us define $A_c^{(k)}$ and $E^{(k)}$ for $k \geq 1$ by

$$A_c^{(k+1)} \equiv (U^{(k)})^H A_c^{(k)} V^{(k)}, \quad E^{(k+1)} \equiv (U^{(k)})^H E^{(k)} V^{(k)},$$

where $A_c^{(1)} = A_c,\ E^{(1)} = E$. Then $A^{(k)} = A_c^{(k)} + E^{(k)}$ and since a two-sided unitary transformation does not change the Frobenius norm of a matrix, $\|E^{(k)}\|_F = \|E\|_F,\ k \geq 1$.

Let us define the gap for clusters by

$$d_c \equiv \min_{i \neq j} |c_i - c_j|, \quad 1 \leq i, j \leq q. \tag{19}$$

Now we formulate asymptotic assumptions for the case of clusters of singular values at the iteration step k.

B1 $\|\mathrm{off}(A^{(k)})\|_F$ and $\|E^{(k)}\|_F = \|E\|_F$ are small quantities:

$$\|\mathrm{off}(A^{(k)})\|_F < \frac{d_c}{8}, \quad \|E^{(k)}\|_F < \frac{d_c}{8}.$$

B2 The main diagonal of $A^{(k)}$ is ordered (e.g., non-increasingly) by suitable row and column permutations so that the diagonal elements of $A^{(k)}$ affiliated with the cluster of singular values $Cl_i,\ 1 \leq i \leq q$, occupy successive positions on the diagonal and can be grouped into the cluster $\widehat{Cl}_i^{(k)},\ 1 \leq i \leq q$.

B3 The partition of $A^{(k)}$ is such that the diagonal elements affiliated with the same cluster Cl_i of singular values are confined to one diagonal block. □

Note that the assumption $\|E^{(k)}\|_F < d_c/8$ is essentially the assumption about the tightness of clusters of A's singular values.

Since $\|E^{(k)}\|_2 \leq \|E^{(k)}\|_F$, **B1** implies

$$Cl_i \subset \left(c_i - \frac{d_c}{8}, c_i + \frac{d_c}{8} \right), \ 1 \leq i \leq q.$$

Our aim is to show that the clusters $\widehat{Cl}_i^{(k)},\ 1 \leq i \leq q$, of diagonal elements of $A^{(k)}$ are stabilized. The approach is similar to that of subsection 1.2.

Lemma 4 *Under assumptions* **B1**–**B3**, *let a cluster* $\widehat{Cl}_i^{(k)},\ 1 \leq i \leq q$, *lie inside the diagonal block* $A_{tt}^{(k)}$ *for some fixed* $t,\ 1 \leq t \leq w$. *Assume that the algorithm uses the LODE in each iteration step. Then, for all iteration steps* $r,\ r \geq k,\ n_i$ *elements of* $\widehat{Cl}_i^{(r)}$ *occupy successive positions on the diagonal inside the same diagonal block* $A_{tt}^{(r)}$. *Consequently, the distance between any two different clusters remains at least* $d_c/2$.

Proof: The proof is identical to that of Lemma 4 in [6]. □

Finally, the value of the constant δ can be identified.

Lemma 5 *For clusters of singular values of A, under assumptions* **B1**–**B3** *above and using the LODE, the constant δ in Theorem 1 can be set to $\delta = \sqrt{2}d_c/4$ where d_c is the gap for clusters defined by Eq. (19).*

Proof: Repeating the proof of Lemma 3, albeit working with c_i and c_j instead of σ_{s_i} and σ_{s_j}, respectively, we get the value $d_c/2$ for the lower bound of distance between spectra of corresponding two diagonal blocks in the Sylvester equation (18). Then repeat the remaining estimates of Lemma 3. □

2 Parallel two-sided SVD algorithm

Let us divide a square matrix A of order n into a $w \times w$ block structure using the blocking factor $w = 2p,\ w \geq 4$, where p is the number of processors. Thus, w denotes the number of blocks in each block row (column) and each block has size $\ell \times \ell$ where $\ell = n/(2p)$. Usually, each processor contains 2 block columns or 2 block rows, but the exact data layout is not significant for the following discussion at all.

At the beginning of a parallel iteration step k, $2p$ off-diagonal blocks of $A^{(k)}$ with block indices (X_{k_1}, Y_{k_1}), (Y_{k_1}, X_{k_1}), $\ldots$, (X_{k_p}, Y_{k_p}), (Y_{k_p}, X_{k_p}), $X_{k_i} < Y_{k_i}$ for all i, are eliminated using the greedy implementation of parallel dynamic ordering (GIPDO). It is appropriate here to briefly recall how the GIPDO works. The pairs of off-diagonal blocks are ordered decreasingly with respect to their weights $w_{IJ}^{(k)}$ measured by the sum of squares of their Frobenius norms,

$$w_{IJ}^{(k)} = \|A_{IJ}^{(k)}\|_F^2 + \|A_{JI}^{(k)}\|_F^2,\ I \neq J.$$

After choosing the first pair, additional $p-1$ pairs are chosen for annihilation with a decreasing weight in a compatible way—i.e., each new pair must have its block-row and block-column indices different from all already chosen blocks. This ensures the selection of p 2×2 block subproblems that can be solved in parallel.

After the GIPDO is computed, p chosen pairs together with corresponding diagonal blocks are met in p processors (one pair per processor), and p 2×2-block SVD subproblems are computed in parallel. At parallel iteration step k, the processor $i,\ 1 \leq i \leq p$, solves the local subproblem of size $2\ell \times 2\ell$,

$$\begin{pmatrix} U_{X_{k,i}X_{k,i}}^{(k)} & U_{X_{k,i}Y_{k,i}}^{(k)} \\ U_{Y_{k,i}X_{k,i}}^{(k)} & U_{Y_{k,i}Y_{k,i}}^{(k)} \end{pmatrix}^H \begin{pmatrix} A_{X_{k,i}X_{k,i}}^{(k)} & A_{X_{k,i}Y_{k,i}}^{(k)} \\ A_{Y_{k,i}X_{k,i}}^{(k)} & A_{Y_{k,i}Y_{k,i}}^{(k)} \end{pmatrix} \begin{pmatrix} V_{X_{k,i}X_{k,i}}^{(k)} & V_{X_{k,i}Y_{k,i}}^{(k)} \\ V_{Y_{k_i}X_{k,i}}^{(k)} & V_{Y_{k,i}Y_{k,i}}^{(k)} \end{pmatrix} = \begin{pmatrix} A_{X_{k,i}X_{k,i}}^{(k+1)} & 0 \\ 0 & A_{Y_{k,i}Y_{k,i}}^{(k+1)} \end{pmatrix},$$

where the diagonal blocks $A_{X_{k,i}X_{k,i}}^{(k+1)}$ and $A_{Y_{k,i}Y_{k,i}}^{(k+1)}$ are square, diagonal matrices of order ℓ, because all diagonal blocks are diagonal after the first parallel iteration step and remain so during the whole computation.

Notice that the matrix

$$U_{k,i}^{(k)} \equiv \begin{pmatrix} U_{X_{k,i}X_{k,i}}^{(k)} & U_{X_{k,i}Y_{k,i}}^{(k)} \\ U_{Y_{k,i}X_{k,i}}^{(k)} & U_{Y_{k,i}Y_{k,i}}^{(k)} \end{pmatrix}$$

is the unitary matrix of left singular vectors, and

$$V_{k,i}^{(k)} \equiv \begin{pmatrix} V_{X_{k,i}X_{k,i}}^{(k)} & V_{X_{k,i}Y_{k,i}}^{(k)} \\ V_{Y_{k,i}X_{k,i}}^{(k)} & V_{Y_{k,i}Y_{k,i}}^{(k)} \end{pmatrix}$$

is the unitary matrix of right singular vectors. The diagonal matrix

$$\Sigma_{k,i}^{(k)} \equiv \begin{pmatrix} A_{X_{k,i}X_{k,i}}^{(k+1)} & 0 \\ 0 & A_{Y_{k,i}Y_{k,i}}^{(k+1)} \end{pmatrix}$$

contains singular values of the matrix

$$A_{k,i}^{(k)} \equiv \begin{pmatrix} A_{X_{k,i}X_{k,i}}^{(k)} & A_{X_{k,i}Y_{k,i}}^{(k)} \\ A_{Y_{k,i}X_{k,i}}^{(k)} & A_{Y_{k,i}Y_{k,i}}^{(k)} \end{pmatrix}.$$

The singular values in any 2×2 block subproblem and in any processor i.e., the elements of $\Sigma_{k,i}^{(k)}$, can be computed and located on the diagonal in any order. An important variant of the local SVD is that with *ordered* singular values (non-increasingly or non-decreasingly). This variant of the SVD of a 2×2 block subproblem will be called the *local ordering of diagonal elements (LODE)*; see also [6].

The proof of global convergence is very similar to the serial case. Since

$$\|\text{off}(A^{(k)})\|_F^2 \leq \frac{w(w-1)}{2}(\|A_{X_{k,1}Y_{k,1}}^{(k)}\|_F^2 + \|A_{Y_{k,1}X_{k,1}}^{(k)}\|_F^2),$$

one has

$$\begin{aligned} \|\text{off}(A^{(k+1)})\|_F^2 &= \|\text{off}(A^{(k)})\|_F^2 - \sum_{i=1}^{p}(\|A_{X_{k,i}Y_{k,i}}^{(k)}\|_F^2 + \|A_{Y_{k,i}X_{k,i}}^{(k)}\|_F^2) \\ &\leq \|\text{off}(A^{(k)})\|_F^2 - (\|A_{X_{k,1}Y_{k,1}}^{(k)}\|_F^2 + \|A_{Y_{k,1}X_{k,1}}^{(k)}\|_F^2) \\ &\leq \left(1 - \frac{2}{w(w-1)}\right)\|\text{off}(A^{(k)})\|_F^2. \end{aligned}$$

2.1 Update of an off-diagonal block

Suppose that in a given parallel iteration step k (its index is omitted here) the off-diagonal blocks $A_{X_iY_i}$ and $A_{Y_iX_i}$ were chosen for annihilation by GIPDO. Our first step is to derive an upper bound for the change of the squared Frobenius norm of an arbitrary block that is not eliminated at parallel step k. Such a block can be written as $A_{X_iX_j}$, $A_{X_iY_j}$, $A_{Y_iX_j}$ or $A_{Y_iY_j}$, where $i \neq j$.

Let us consider the update of block rows X_i and Y_i. We need to evaluate the update of two off-diagonal blocks which will be combined in the subsequent update of two block columns:

$$\begin{aligned}\tilde{A}_{X_iX_j} &= U^H_{X_iX_i}A_{X_iX_j} + U^H_{Y_iX_i}A_{Y_iX_j},\\ \tilde{A}_{X_iY_j} &= U^H_{X_iX_i}A_{X_iY_j} + U^H_{Y_iX_i}A_{Y_iY_j}.\end{aligned} \tag{20}$$

Secondly, the update of two block columns X_j, Y_j follows from Eq. (20):

$$\begin{aligned}\hat{A}_{X_iX_j} &= \tilde{A}_{X_iX_j}V_{X_jX_j} + \tilde{A}_{X_iY_j}V_{Y_jX_j}\\ &= U^H_{X_iX_i}A_{X_iX_j}V_{X_jX_j} + U^H_{Y_iX_i}A_{Y_iX_j}V_{X_jX_j}\\ &\quad + U^H_{X_iX_i}A_{X_iY_j}V_{Y_jX_j} + U^H_{Y_iX_i}A_{Y_iY_j}V_{Y_jX_j}.\end{aligned}$$

In the following lemma, we bound the change of $A_{X_iX_j}$, but the same bound is applicable to other three cases as well.

Lemma 6 *Consider the change of an off-diagonal block $A_{X_iX_j}$ that was not eliminated in a given parallel iteration step k. Denote the changed block by $\hat{A}_{X_iX_j}$, and let $C_i = (A_{X_iY_i}, A_{Y_iX_i})$. Additionally, let A_{ST} be the off-diagonal block with the largest Frobenius norm, $\|A_{ST}\|_F = \max_{I\neq J}\|A_{IJ}\|_F$. If there exists a constant $\delta > 0$ such that $\left\|\begin{pmatrix} U_{Y_iX_i}\\ V_{Y_iX_i}\end{pmatrix}\right\|_2 \leq \|C_i\|_F/\delta$ for $1 \leq i \leq p$, then the following inequality holds:*

$$\begin{aligned}\left|\|\hat{A}_{X_iX_j}\|_F^2 - \|A_{X_iX_j}\|_F^2\right| &\leq \frac{\|A_{ST}\|_F^2}{\delta^2}\left\{(1+\sqrt{2})\|C_i\|_F^2 + (2+\sqrt{2})\|C_j\|_F^2\right\}\\ &\quad + 2\,\frac{\|A_{ST}\|_F}{\delta}\left(\|C_i\|_F + \sqrt{2}\|C_j\|_F\right)\|A_{X_iX_j}\|_F.\end{aligned} \tag{21}$$

Proof: Using the triangle inequality, we can bound the left-hand side of Eq. (21) as

$$\left|\|\hat{A}_{X_iX_j}\|_F^2 - \|A_{X_iX_j}\|_F^2\right| \leq \left|\|\tilde{A}_{X_iX_j}\|_F^2 - \|A_{X_iX_j}\|_F^2\right| + \left|\|\hat{A}_{X_iX_j}\|_F^2 - \|\tilde{A}_{X_iX_j}\|_F^2\right|. \tag{22}$$

Using Eq. (20), the first term in the right-hand side can be bounded using the same technique as in the proof of Lemma 1 of [6] as

$$\begin{aligned}&\left|\|\tilde{A}_{X_iX_j}\|_F^2 - \|A_{X_iX_j}\|_F^2\right|\\ &\leq \|U_{Y_iX_i}\|_2^2\max\left\{\|A_{X_iX_j}\|_F^2, \|A_{Y_iX_j}\|_F^2\right\} + 2\|A_{X_iX_j}\|_F\|U_{Y_iX_i}\|_2\|A_{Y_iX_j}\|_F\\ &\leq \frac{\|A_{ST}\|_F^2}{\delta^2}\|C_i\|_F^2 + 2\,\frac{\|A_{ST}\|_F}{\delta}\|C_i\|_F\|A_{X_iX_j}\|_F.\end{aligned} \tag{23}$$

Similarly, the second term can be bounded as

$$\begin{aligned}&\left|\|\hat{A}_{X_iX_j}\|_F^2 - \|\tilde{A}_{X_iX_j}\|_F^2\right|\\ &\leq \|V_{Y_jX_j}\|_2^2\max\left\{\|\tilde{A}_{X_iX_j}\|_F^2, \|\tilde{A}_{X_iY_j}\|_F^2\right\} + 2\|\tilde{A}_{X_iX_j}\|_F\|V_{Y_jX_j}\|_2\|\tilde{A}_{X_iY_j}\|_F.\end{aligned} \tag{24}$$

To bound the right-hand side, we need to evaluate $\|\tilde{A}_{X_iX_j}\|_F$ and $\|\tilde{A}_{X_iY_j}\|_F$. Using again Eq. (20), we have

$$\begin{aligned}\|\tilde{A}_{X_iX_j}\|_F &\leq \|A_{X_iX_j}\|_F + \|U_{Y_iX_i}\|_2\|A_{Y_iX_j}\|_F\\ &\leq \|A_{X_iX_j}\|_F + \frac{\|C_i\|_F}{\delta}\|A_{ST}\|_F.\end{aligned} \tag{25}$$

On the other hand, since the transformation is unitary, we have

$$\|\tilde{A}_{X_iX_j}\|_F^2 + \|\tilde{A}_{Y_iX_j}\|_F^2 = \|A_{X_iX_j}\|_F^2 + \|A_{Y_iX_j}\|_F^2,$$

which leads to

$$\|\tilde{A}_{X_iX_j}\|_F^2 \le \|A_{X_iX_j}\|_F^2 + \|A_{Y_iX_j}\|_F^2 \le 2\|A_{ST}\|_F^2. \tag{26}$$

Similarly,

$$\|\tilde{A}_{X_iY_j}\|_F^2 \le \|A_{X_iY_j}\|_F^2 + \|A_{Y_iY_j}\|_F^2 \le 2\|A_{ST}\|_F^2. \tag{27}$$

Putting Eqs. (26) and (27) into the first term of Eq. (24) and putting Eq. (25) and (27) into the second term of Eq. (24) gives

$$\begin{aligned}
&\left|\|\hat{A}_{X_iX_j}\|_F^2 - \|\tilde{A}_{X_iX_j}\|_F^2\right| \\
&\le \frac{\|C_j\|_F^2}{\delta^2}\cdot 2\|A_{ST}\|_F^2 + 2\left(\|A_{X_iX_j}\|_F + \frac{\|C_i\|_F}{\delta}\|A_{ST}\|_F\right)\cdot\frac{\|C_j\|_F}{\delta}\cdot\sqrt{2}\|A_{ST}\|_F \\
&= 2\,\frac{\|A_{ST}\|_F^2}{\delta^2}\left(\|C_j\|_F^2 + \sqrt{2}\,\|C_i\|_F\|C_j\|_F\right) + 2\sqrt{2}\,\frac{\|A_{ST}\|_F}{\delta}\,\|C_j\|_F\|A_{X_iX_j}\|_F \\
&\le \frac{\|A_{ST}\|_F^2}{\delta^2}\left\{2\|C_j\|_F^2 + \sqrt{2}\left(\|C_i\|_F^2 + \|C_j\|_F^2\right)\right\} \\
&\quad +2\sqrt{2}\,\frac{\|A_{ST}\|_F}{\delta}\,\|C_j\|_F\|A_{X_iX_j}\|_F,
\end{aligned} \tag{28}$$

where we used $2ab \le a^2 + b^2$ in the last inequality. Substituting Eqs. (23) and (28) into (22) leads to

$$\begin{aligned}
\left|\|\hat{A}_{X_iX_j}\|_F^2 - \|A_{X_iX_j}\|_F^2\right| \;\le\; & \frac{\|A_{ST}\|_F^2}{\delta^2}\left\{(1+\sqrt{2})\|C_i\|_F^2 + (2+\sqrt{2})\|C_j\|_F^2\right\} \\
& +2\,\frac{\|A_{ST}\|_F}{\delta}\left(\|C_i\|_F + \sqrt{2}\|C_j\|_F\right)\|A_{X_iX_j}\|_F,
\end{aligned}$$

which completes the proof. □

2.2 Asymptotic quadratic convergence

Using Lemma 6, we derive a quadratic convergence bound for the parallel block Jacobi SVD algorithm with GIPDO.

Theorem 2 *Consider the parallel two-sided block-Jacobi SVD algorithm with GIPDO using the blocking factor $w = 2p$. Without loss of generality, denote the parallel iteration steps by $k = 0, 1, \ldots,$ and the off-diagonal blocks chosen for elimination at step k by $A^{(k)}_{X_{k,1}Y_{k,1}}, A^{(k)}_{Y_{k,1}X_{k,1}}, \ldots, A^{(k)}_{X_{k,p}Y_{k,p}}, A^{(k)}_{Y_{k,p}X_{k,p}}$, where $A^{(k)}_{X_{k,1}Y_{k,1}}$ and $A^{(k)}_{Y_{k,1}X_{k,1}}$ are the off-diagonal blocks that give the largest weight. Let $A^{(k)}_{S_kT_k}$ be the off-diagonal block with the largest Frobenius norm. Additionally, let $C^{(k)}_{k,i} = (A^{(k)}_{X_{k,i}Y_{k,i}}, A^{(k)}_{Y_{k,i}X_{k,i}})$, $1 \le i \le p$, and let $\mathcal{Q}_{k,\ell}$, ℓ even, be the index set of the $\ell/2$ pairs of* *off-diagonal blocks with smallest weights at step k (notice that they are chosen in a symmetric way—i.e., if* $(I,J) \in \mathcal{Q}_{k,\ell}$*, then* $(J,I) \in \mathcal{Q}_{k,\ell}$*). Define the index set* $\mathcal{P}_k$ *recursively as follows:*

$$\begin{aligned} \mathcal{P}_0 &= \emptyset, \\ \mathcal{P}_{k+1} &= \mathcal{Q}_{k,|\mathcal{P}_k|} \cup \{(X_{k,1},Y_{k,1}),(Y_{k,1},X_{k,1}),\ldots,(X_{k,p},Y_{k,p}),(Y_{k,p},X_{k,p})\}\,, \end{aligned} \tag{29}$$

where $|\mathcal{P}_k|$ *denotes the number of elements in* $\mathcal{P}_k$*. Then there exists a step* W*,* $w-1 \le W \le w(w-2)/2+1$*, for which* $\mathcal{P}_W$ *equals the set of indices of all off-diagonal blocks. Furthermore, suppose that there exists a constant* $\delta > 0$ *such that* $\left\| \begin{pmatrix} U^{(k)}_{Y_{k,i}X_{k,i}} \\ V^{(k)}_{Y_{k,i}X_{k,i}} \end{pmatrix} \right\|_2 \le \|C^{(k)}_{k,i}\|_F/\delta$ *holds for all* $1 \le i \le p$ *and* $k = 0,1,\ldots,W-1$*. Then,*

$$\|\mathrm{off}(A^{(W)})\|_F^2 \le 3(w-2)\left(\frac{2\|\mathrm{off}(A^{(0)})\|_F^2}{\delta}\right)^2, \tag{30}$$

that is, the parallel two-sided block-Jacobi SVD algorithm with the GIPDO converges quadratically after W *iterations.*

Proof: We first show the existence of W. From the definition, $\mathcal{P}_1 = \{(X_{0,1},Y_{0,1}),(Y_{0,1},X_{0,1}), \ldots, (X_{0,p},Y_{0,p}),(Y_{0,p},X_{0,p})\}$, so $|\mathcal{P}_1| = 2p = w$. Assume that $|\mathcal{P}_k| < w(w-1)$, the number of off-diagonal blocks, for some $k \ge 1$. Then, actually $\mathcal{P}_k \le w(w-1)-2$ because $\mathcal{P}_k$ has even number of elements by construction. This means that $(X_{k,1},Y_{k,1})$ and $(Y_{k,1},X_{k,1})$, which are the indices of off-diagonal blocks with the largest weight, do not belong to $\mathcal{Q}_{k,|\mathcal{P}_k|}$. Thus, $\mathcal{P}_{k+1}$ has at least two more elements than $\mathcal{Q}_{k,|\mathcal{P}_k|}$ and $|\mathcal{P}_{k+1}| \ge |\mathcal{Q}_{k,|\mathcal{P}_k|}| + 2 = |\mathcal{P}_k| + 2$. On the other hand, it is clear from Eq. (29) that $|\mathcal{P}_{k+1}| \le |\mathcal{Q}_{k,|\mathcal{P}_k|}| + 2p = |\mathcal{P}_k| + 2p$. Hence, the increase in the number of elements of $\mathcal{P}_k$ at each step is between 2 and $2p$. In the *worst case* scenario, the increase at each step is constantly 2, so $|\mathcal{P}'_k| = 2p + 2(k-1)$ for $k = 1,2,\ldots$. In this case, $|\mathcal{P}_k| = w(w-1)$ is reached at step $k = w(w-2)/2+1$. In the *best case* scenario, in which

$$\mathcal{Q}_{k,|\mathcal{P}_k|} \cap \{(X_{k,1},Y_{k,1}),(Y_{k,1},X_{k,1}),\ldots,(X_{k,p},Y_{k,p}),(Y_{k,p},X_{k,p})\} = \emptyset$$

holds at every step, $|\mathcal{P}'_k| = 2kp$ for $k = 1,2,\ldots$. In this case, $|\mathcal{P}_k| = w(w-1)$ is reached at step $k = w-1$. Other cases are in between.

To prove Eq. (30), we show an alternative inequality

$$\sum_{(I,J)\in\mathcal{P}_k} \|A^{(k)}_{IJ}\|_F^2 \le \left(\frac{2+\sqrt{2}}{2}\right)^2 (w-2)\left(\frac{2\|\mathrm{off}(A^{(0)})\|_F^2 - 2\|\mathrm{off}(A^{(k)})\|_F^2}{\delta}\right)^2 \tag{31}$$

for $k = 0,1,\ldots,W$. Note that when $k = W$, the left-hand side becomes $\|\mathrm{off}(A^{(W)})\|_F^2$, while the right-hand side is smaller than the right-hand side of Eq. (30). So Eq. (30) follows directly from Eq. (31). We prove Eq. (31) by induction. When $k = 0$, both sides are zero, so the inequality holds trivially. We assume that Eq. (31) holds for some $k < W$ and show that it also holds for $k+1$. In the following, we omit the superscript (k) for the parallel iteration step and denote the quantities at step k and $k+1$ by symbols without and with a hat, respectively. We also write $C^{(k)}_{k,i}$, $X_{k,i}$ and $Y_{k,i}$ as C_i, X_i and Y_i, respectively.

Let us define the index set $\mathcal{P}'_k$ by

$$\mathcal{P}'_k = \mathcal{Q}_{k,|\mathcal{P}_k|} \setminus \{(X_1,Y_1),(Y_1,X_1),\ldots,(X_p,Y_p),(Y_p,X_p)\}\,. \tag{32}$$

Then, the left-hand side of Eq. (31) at parallel step $k+1$ can be evaluated as follows:

$$\begin{aligned}\sum_{(I,J)\in\mathcal{P}_{k+1}} \|\hat{A}_{IJ}\|_F^2 &= \sum_{(I,J)\in\mathcal{P}'_k} \|\hat{A}_{IJ}\|_F^2 + \sum_{i=1}^{p}(\|\hat{A}_{X_iY_i}\|_F^2 + \|\hat{A}_{Y_iX_i}\|_F^2) \\ &\le \sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}\|_F^2 + \sum_{(I,J)\in\mathcal{P}'_k} \left| \|\hat{A}_{IJ}\|_F^2 - \|A_{IJ}\|_F^2 \right|, \end{aligned} \tag{33}$$

where we used $\|\hat{A}_{X_iY_i}\|_F^2 = \|\hat{A}_{Y_iX_i}\|_F^2 = 0$ for $1 \le i \le p$.

Let $(I,J) \in \mathcal{P}'_k$ be fixed. Since $\{X_1, Y_1, \ldots, X_p, Y_p\}$ is a permutation of $\{1, 2, \ldots, 2p\}$, for each I, there exists exactly one index i $(1 \le i \le p)$ such that $I = X_i$ or $I = Y_i$. We denote such i by $\pi(I)$. Using the same mapping π, we can denote the index j $(1 \le j \le p)$ such that $J = X_j$ or $J = Y_j$ by $\pi(J)$. Then, the off-diagonal block A_{IJ} is updated by a block rotation specified by $(X_{\pi(I)}, Y_{\pi(I)})$ from the left and by another block rotation specified by $(X_{\pi(J)}, Y_{\pi(J)})$ from the right. Note that $\pi(I) \ne \pi(J)$, because A_{IJ} is not a block chosen for elimination. Hence, we have from Eq. (21),

$$\begin{aligned}\left| \|\hat{A}_{IJ}\|_F^2 - \|A_{IJ}\|_F^2 \right| &\le 2\,\frac{\|A_{ST}\|_F}{\delta}\,(\|C_{\pi(I)}\|_F + \sqrt{2}\,\|C_{\pi(J)}\|_F)\|A_{IJ}\|_F \\ &\quad + \frac{\|A_{ST}\|_F^2}{\delta^2}\left\{(1+\sqrt{2})\|C_{\pi(I)}\|_F^2 + (2+\sqrt{2})\|C_{\pi(J)}\|_F^2\right\}. \end{aligned} \tag{34}$$

Now, consider the sum of $\|C_{\pi(I)}\|_F^2$ over $\mathcal{P}'_k$. Since $\mathcal{P}'_k \subseteq \{(I,J) \,|\, 1 \le I, J \le 2p,\ \pi(I) \ne \pi(J)\}$, we can bound it by a sum over the set $\{(I,J) \,|\, 1 \le I, J \le 2p,\ \pi(I) \ne \pi(J)\}$. Furthermore, there exist exactly two values of I such that $\pi(I) = i$ for each i and exactly two values of J such that $\pi(J) = j$ for each j. Hence, we can rewrite the sum over the set $\{(I,J) \,|\, 1 \le I, J \le 2p,\ \pi(I) \ne \pi(J)\}$ as a sum over the set $\{(i,j) \,|\, 1 \le i, j \le p,\ i \ne j\}$ multiplied by 4. Thus,

$$\begin{aligned}\sum_{(I,J)\in\mathcal{P}'_k} \|C_{\pi(I)}\|_F^2 &\le \sum_{I=1}^{2p} \sum_{\substack{J=1 \\ \pi(I)\ne\pi(J)}}^{2p} \|C_{\pi(I)}\|_F^2 \\ &= 4\sum_{i=1}^{p} \sum_{\substack{j=1 \\ j\ne i}}^{p} \|C_i\|_F^2 \\ &= 4(p-1)\sum_{i=1}^{p} \|C_i\|_F^2 = 2(w-2)\sum_{i=1}^{p} \|C_i\|_F^2. \end{aligned} \tag{35}$$

Similarly,

$$\sum_{(I,J)\in\mathcal{P}'_k} \|C_{\pi(J)}\|_F^2 \le 2(w-2)\sum_{i=1}^{p} \|C_i\|_F^2. \tag{36}$$

Using these results, we can now bound the second term in the right-hand side of Eq. (33). By inserting Eq. (34) into Eq. (33), we have

$$\begin{aligned}
&\sum_{(I,J)\in\mathcal{P}'_k} \left| \|\hat{A}_{IJ}\|_F^2 - \|A_{IJ}\|_F^2 \right| \\
&\leq \frac{\|A_{ST}\|_F}{\delta} \sum_{(I,J)\in\mathcal{P}'_k} (2\,\|C_{\pi(I)}\|_F + 2\sqrt{2}\,\|C_{\pi(J)}\|_F)\|A_{IJ}\|_F \\
&\quad + \frac{\|A_{ST}\|_F^2}{\delta^2} \sum_{(I,J)\in\mathcal{P}'_k} \left\{ (1+\sqrt{2})\|C_{\pi(I)}\|_F^2 + (2+\sqrt{2})\|C_{\pi(J)}\|_F^2 \right\} \\
&\leq \frac{\|A_{ST}\|_F}{\delta} \left(2\sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|C_{\pi(I)}\|_F^2} + 2\sqrt{2}\sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|C_{\pi(J)}\|_F^2} \right) \sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}\|_F^2} \\
&\quad + \frac{\|A_{ST}\|_F^2}{\delta^2} \left\{ (1+\sqrt{2}) \sum_{(I,J)\in\mathcal{P}'_k} \|C_{\pi(I)}\|_F^2 + (2+\sqrt{2}) \sum_{(I,J)\in\mathcal{P}'_k} \|C_{\pi(J)}\|_F^2 \right\} \\
&\leq \frac{1}{\delta} \sqrt{\sum_{i=1}^{p} \|C_i\|_F^2} \cdot (4+2\sqrt{2})\sqrt{w-2} \sqrt{\sum_{i=1}^{p} \|C_i\|_F^2} \sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}\|_F^2} \\
&\quad + \frac{1}{\delta^2} \left(\sum_{i=1}^{p} \|C_i\|_F^2 \right) \cdot (6+4\sqrt{2})(w-2) \left(\sum_{i=1}^{p} \|C_i\|_F^2 \right) \\
&= \frac{2(2+\sqrt{2})\sqrt{w-2}}{\delta} \left(\sum_{i=1}^{p} \|C_i\|_F^2 \right) \sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}\|_F^2} \\
&\quad + \frac{(2+\sqrt{2})^2(w-2)}{\delta^2} \left(\sum_{i=1}^{p} \|C_i\|_F^2 \right)^2 ,
\end{aligned} \tag{37}$$

where we used the Cauchy-Schwarz inequality in the second inequality. In the third inequality, we used

$$\begin{aligned}
\|A_{ST}\|_F &\leq \sqrt{\|A_{ST}\|_F^2 + \|A_{TS}\|_F^2} \leq \sqrt{\|A_{X_1Y_1}\|_F^2 + \|A_{Y_1X_1}\|_F^2} \\
&\leq \sqrt{\sum_{i=1}^{p} (\|A_{X_iY_i}\|_F^2 + \|A_{Y_iX_i}\|_F^2)} = \sqrt{\sum_{i=1}^{p} \|C_i\|_F^2}
\end{aligned}$$

to bound the first factor of the first and second term, and Eqs. (35) and (36) to bound the sums over $\mathcal{P}'_k$. Inserting Eq. (37) into Eq. (33) finally gives:

$$\begin{aligned}
\sum_{(I,J)\in\mathcal{P}_{k+1}} \|\hat{A}_{IJ}\|_F^2 &\leq \sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}\|_F^2 + \frac{2(2+\sqrt{2})\sqrt{w-2}}{\delta}\left(\sum_{i=1}^{p}\|C_i\|_F^2\right)\sqrt{\sum_{(I,J)\in\mathcal{P}'_k}\|A_{IJ}\|_F^2} \\
&\quad + \frac{(2+\sqrt{2})^2(w-2)}{\delta^2}\left(\sum_{i=1}^{p}\|C_i\|_F^2\right)^2 \\
&= \left\{\sqrt{\sum_{(I,J)\in\mathcal{P}'_k}\|A_{IJ}\|_F^2} + \frac{(2+\sqrt{2})\sqrt{w-2}}{2\delta}\cdot 2\sum_{i=1}^{p}\|C_i\|_F^2\right\}^2 \\
&\leq \left(\frac{2+\sqrt{2}}{2}\right)^2 (w-2)\left(\frac{2\|\mathrm{off}(A^{(0)})\|_F^2 - 2\|\mathrm{off}(A^{(k)})\|_F^2 + 2\sum_{i=1}^{p}\|C_i\|_F^2}{\delta}\right)^2 \\
&= \left(\frac{2+\sqrt{2}}{2}\right)^2 (w-2)\left(\frac{2\|\mathrm{off}(A^{(0)})\|_F^2 - 2\|\mathrm{off}(A^{(k+1)})\|_F^2}{\delta}\right)^2, \qquad (38)
\end{aligned}$$

where we used, in the third inequality, the induction assumption given by Eq. (31):

$$\begin{aligned}
\sqrt{\sum_{(I,J)\in\mathcal{P}'_k}\|A_{IJ}\|_F^2} &\leq \sqrt{\sum_{(I,J)\in\mathcal{Q}_{k,|\mathcal{P}_k|}}\|A_{IJ}\|_F^2} \\
&\leq \sqrt{\sum_{(I,J)\in\mathcal{P}_k}\|A_{IJ}\|_F^2} \\
&\leq \frac{2+\sqrt{2}}{2}\sqrt{w-2}\cdot\frac{2\|\mathrm{off}(A^{(0)})\|_F^2 - 2\|\mathrm{off}(A^{(k)})\|_F^2}{\delta}.
\end{aligned}$$

The last equality follows from

$$2\|\mathrm{off}(A^{(k+1)})\|_F^2 = 2\|\mathrm{off}(A^{(k)})\|_F^2 - 2\sum_{i=1}^{p}\|C_i\|_F^2.$$

Hence, Eq. (38) shows that the induction assumption holds also for $k+1$. □

Theorem 2 states that the quadratic reduction of the off-norm occurs after $w(w-2)/2+1$ parallel iterations, at the latest. This is the *worst case* scenario, for which the number of iterations required for quadratic convergence is almost the same as that for the serial algorithm. On the other hand, in the *best case* scenario, the quadratic convergence occurs after only $w-1$ steps. In this case, the number of iterations required for quadratic convergence is $w/2 = p$ times smaller than that for the serial algorithm.

The identification of a constant δ is the same as for serial algorithm. Hence, under assumptions **A1**–**A3** (or **B1**–**B3**) for well-separated singular values (or clusters) made in Section 1, it is $\delta = \sqrt{2}d/4$ (or $\delta = \sqrt{2}d_c/4$).

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