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Abstract. *This report is devoted to the proof of the local (asymptotic) quadratic convergence of the parallel block-Jacobi EVD algorithm for Hermitian matrices with a general spectrum. Individual 2×2 block subproblems are chosen using the parallel dynamic ordering (its greedy implementation) [1]. The upper bound from [4] was improved and no assumption about simple eigenvalues was necessary.*

1 Update of an off-diagonal block

Let us divide a square, Hermitian matrix A of order n into a $w \times w$ block structure using the blocking factor $w = 2p$, 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 $\ell = n/(2p)$.

At parallel iteration step k, $2p$ off-diagonal blocks of $A^{(k)}$ with block indices (X_1, Y_1), (Y_1, X_1), $\dots$, (X_p, Y_p), (Y_p, X_p), $X_i < Y_i$ for all i, are eliminated using the greedy implementation of parallel dynamic ordering (GIPDO). It is appropriate here to recall how the GIPDO works. At the beginning of parallel iteration step k, the pairs of the off-diagonal blocks are ordered decreasingly with respect to their weights,

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

Since the matrix is Hermitian, this ordered list starts with the pair of 'heaviest' blocks which is chosen as the first one for annihilation,

$$\|A_{X_1Y_1}^{(k)}\|_F^2 = \|A_{Y_1X_1}^{(k)}\|_F^2 = \max_{I \neq J} \|A_{IJ}^{(k)}\|_F^2. \tag{1}$$

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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. More details can be found in [1].

At iteration step k, the processor i, $1 \leq i \leq p$, solves the local 2×2-block EVD subproblem

$$\begin{pmatrix} P^{(k)}_{X_{k_i}X_{k_i}} & P^{(k)}_{X_{k_i}Y_{k_i}} \\ P^{(k)}_{Y_{k_i}X_{k_i}} & P^{(k)}_{Y_{k_i}Y_{k_i}} \end{pmatrix}^H \begin{pmatrix} A^{(k)}_{X_{k_i}X_{k_i}} & A^{(k)}_{X_{k_i}Y_{k_i}} \\ A^{(k)}_{Y_{k_i}X_{k_i}} & A^{(k)}_{Y_{k_i}Y_{k_i}} \end{pmatrix} \begin{pmatrix} P^{(k)}_{X_{k_i}X_{k_i}} & P^{(k)}_{X_{k_i}Y_{k_i}} \\ P^{(k)}_{Y_{k_i}X_{k_i}} & P^{(k)}_{Y_{k_i}Y_{k_i}} \end{pmatrix} = \begin{pmatrix} \hat{A}^{(k+1)}_{X_{k_i}X_{k_i}} & 0 \\ 0 & \hat{A}^{(k+1)}_{Y_{k_i}Y_{k_i}} \end{pmatrix}, \quad (2)$$

where the diagonal blocks $\hat{A}^{(k+1)}_{X_{k_i}X_{k_i}}$ and $\hat{A}^{(k+1)}_{Y_{k_i}Y_{k_i}}$ are square, diagonal matrices of order $\ell = n/w$. Notice that the matrix

$$P^{(k)}_{k_i} \equiv \begin{pmatrix} P^{(k)}_{X_{k_i}X_{k_i}} & P^{(k)}_{X_{k_i}Y_{k_i}} \\ P^{(k)}_{Y_{k_i}X_{k_i}} & P^{(k)}_{Y_{k_i}Y_{k_i}} \end{pmatrix} \quad (3)$$

is the unitary matrix of eigenvectors of the matrix

$$A^{(k)}_{k_i} \equiv \begin{pmatrix} A^{(k)}_{X_{k_i}X_{k_i}} & A^{(k)}_{X_{k_i}Y_{k_i}} \\ A^{(k)}_{Y_{k_i}X_{k_i}} & A^{(k)}_{Y_{k_i}Y_{k_i}} \end{pmatrix}. \quad (4)$$

Obviously, the GIPDO may not choose $2p$ largest off-diagonal blocks, because some of them can lie in one block-row or block-column. So, going through the ordered list of weights, the 'jumps' may arise, and, in the worst case, also quite small blocks can be chosen for annihilation from bottom of the ordered list.

Now we are interested in the change of a given off-diagonal block in one parallel iteration step which was not eliminated. The index of the parallel iteration step k is omitted. We will work with two important assumptions:

A1 There exists a constant $\delta > 0$ such that $\|\mathrm{off}(A)\|_F \leq \delta$.

A2 The same constant $\delta > 0$ bounds the spectral norms of submatrices of unitary transformations for all parallel iteration steps starting from step k:

$$\|P_{Y_iX_i}\|_2 = \|P_{X_iY_i}\|_2 \leq \frac{\|A_{X_1Y_1}\|_F}{\delta}, \quad 1 \leq i \leq p.$$

□

Notice that the assumption **A1** is natural because, as shown in [4], the off-diagonal Frobenius norm of $A^{(k)}$ converges to zero in the parallel block-Jacobi EVD algorithm with GIPDO. The assumption **A2** is taken from [3] (see also Remark 1).

In contrast to the serial algorithm, one parallel iteration step changes *all* off-diagonal blocks by two different unitary transformations. Take A_{IJ}, $I \neq J$, $(I,J) \neq (X_i, Y_i)$ and $(I,J) \neq (Y_i, X_i)$ for all i, i.e. A_{IJ} is not eliminated in the parallel iteration step k. Then there exists exactly one unitary transformation from p transformations which changes block rows X_i, Y_i and $I = X_i$

(or $I = Y_i$). Similarly, there exists exactly one unitary transformation from p transformations which changes block columns X_j, Y_j, $j \neq i$, and $J = X_j$ (or $J = Y_j$). In the following we work with $A_{IJ} = A_{X_iX_j}$; other possibilities can be treated in the same way.

Firstly, let us consider the update of block rows X_i, 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:

$$\begin{aligned}\tilde{A}_{X_iX_j} &= P^H_{X_iX_i}A_{X_iX_j} + P^H_{Y_iX_i}A_{Y_iX_j},\\ \tilde{A}_{X_iY_j} &= P^H_{X_iX_i}A_{X_iY_j} + P^H_{Y_iX_i}A_{Y_iY_j}.\end{aligned} \tag{5}$$

Secondly, the update of two block columns X_j, Y_j follows from Eq. (5):

$$\begin{aligned}\hat{A}_{X_iX_j} &= \tilde{A}_{X_iX_j}P_{X_jX_j} + \tilde{A}_{X_iY_j}P_{Y_jX_j}\\ &= P^H_{X_iX_i}A_{X_iX_j}P_{X_jX_j} + P^H_{Y_iX_i}A_{Y_iX_j}P_{X_jX_j}\\ &\quad + P^H_{X_iX_i}A_{X_jY_j}P_{Y_jX_j} + P^H_{Y_iX_i}A_{Y_iY_j}P_{Y_jX_j}.\end{aligned} \tag{6}$$

Next, the upper bound for the change $\left| \|\hat{A}_{X_iX_j}\|_F^2 - \|A_{X_iX_j}\|_F^2 \right|$ will be estimated. Recall that $\|A\|_F^2 = \mathrm{Tr}(A^HA)$ and $|\mathrm{Tr}(A^HB)| \leq \|A\|_F \, \|B\|_F$ for any matrix A and any compatible matrix pair A, B, where $\mathrm{Tr}(\cdot)$ is the trace operator. Based on Eqs. (5) and (6),

$$\begin{aligned}&\left| \|\hat{A}_{X_iX_j}\|_F^2 - \|A_{X_iX_j}\|_F^2 \right| =\\ &= \big| \|P^H_{X_iX_i}A_{X_iX_j}P_{X_jX_j} + P^H_{Y_iX_i}A_{Y_iX_j}P_{X_jX_j} + P^H_{X_iX_i}A_{X_jY_j}P_{Y_jX_j} + P^H_{Y_iX_i}A_{Y_iY_j}P_{Y_jX_j}\|_F^2 -\\ &\qquad - \|A_{X_iX_j}\|_F^2 \big|\\ &\leq \underbrace{\big| \|A_{X_iX_j}\|_F^2 - \|P^H_{X_iX_i}A_{X_iX_j}P_{X_jX_j}\|_F^2 - \|P^H_{Y_iX_i}A_{Y_iX_j}P_{X_jX_j}\|_F^2 \big|}_{|\mathrm{Term1}|}\\ &+ \underbrace{\|P^H_{X_iX_i}A_{X_jY_j}P_{Y_jX_j}\|_F^2 + \|P^H_{Y_iX_i}A_{Y_iY_j}P_{Y_jX_j}\|_F^2}_{\mathrm{Term2}}\\ &+ \underbrace{\left| \mathrm{Tr}\left[\left(P^H_{X_iX_i}A_{X_iX_j}P_{X_jX_j}\right)^H \left(P^H_{Y_iX_i}A_{Y_iX_j}P_{X_jX_j} + P^H_{X_iX_i}A_{X_jY_j}P_{Y_jX_j} + P^H_{Y_iX_i}A_{Y_iY_j}P_{Y_jX_j}\right)\right]\right|}_{|\mathrm{Tr}_1|}\\ &+ \underbrace{\left| \mathrm{Tr}\left[\left(P^H_{Y_iX_i}A_{Y_iX_j}P_{X_jX_j}\right)^H \left(P^H_{X_iX_i}A_{X_iX_j}P_{X_jX_j} + P^H_{X_iX_i}A_{X_jY_j}P_{Y_jX_j} + P^H_{Y_iX_i}A_{Y_iY_j}P_{Y_jX_j}\right)\right]\right|}_{|\mathrm{Tr}_2|}\\ &+ \underbrace{\left| \mathrm{Tr}\left[\left(P^H_{X_iX_i}A_{X_jY_j}P_{Y_jX_j}\right)^H \left(P^H_{X_iX_i}A_{X_iX_j}P_{X_jX_j} + P^H_{Y_iX_i}A_{Y_iX_j}P_{X_jX_j} + P^H_{Y_iX_i}A_{Y_iY_j}P_{Y_jX_j}\right)\right]\right|}_{|\mathrm{Tr}_3|}\\ &+ \underbrace{\left| \mathrm{Tr}\left[\left(P^H_{Y_iX_i}A_{Y_iY_j}P_{Y_jX_j}\right)^H \left(P^H_{X_iX_i}A_{X_iX_j}P_{X_jX_j} + P^H_{Y_iX_i}A_{Y_iX_j}P_{X_jX_j} + P^H_{X_iX_i}A_{X_jY_j}P_{Y_jX_j}\right)\right]\right|}_{|\mathrm{Tr}_4|}.\end{aligned} \tag{7}$$

Last six rows of Eq. (7) will be bounded separately. Firstly, notice that

$$\|P^H_{X_iX_i}A_{X_iX_j}P_{X_jX_j}\|_F^2 \leq \|P_{X_iX_i}\|_2^2 \, \|P_{X_jX_j}\|_2^2 \, \|A_{X_iX_j}\|_F^2 \leq \|A_{X_iX_j}\|_F^2,$$

since $\|P_{X_sX_s}\|_2 \leq 1$, $s = i, j$, from the Cosine-Sine decomposition (CSD) of the unitary matrix

P_i. Hence, $\|A_{X_iX_j}\|_F^2 - \|P_{X_iX_i}^H A_{X_iX_j} P_{X_jX_j}\|_F^2 \geq 0$. Moreover, from the same CSD,

$$\begin{aligned}
\|P_{X_iX_i}^H A_{X_iX_j} P_{X_jX_j}\|_F^2 &\geq \sigma_{\min}^2(P_{X_iX_i})\, \sigma_{\min}^2(P_{X_jX_j})\, \|A_{X_iX_j}\|_F^2 \\
&= (1 - \|P_{Y_iX_i}\|_2^2)\,(1 - \|P_{Y_jX_j}\|_2^2)\, \|A_{X_iX_j}\|_F^2 \\
&= \big(1 - \|P_{Y_iX_i}\|_2^2 - \|P_{Y_jX_j}\|_2^2 + \|P_{Y_iX_i}\|_2^2\, \|P_{Y_jX_j}\|_2^2\big)\, \|A_{X_iX_j}\|_F^2 \geq 0.
\end{aligned} \tag{8}$$

Now we proceed with individual bounds in Eq. (7):

$$\begin{aligned}
|\text{Term1}| &= \big|\big(\|A_{X_iX_j}\|_F^2 - \|P_{X_iX_i}^H A_{X_iX_j} P_{X_jX_j}\|_F^2\big) - \|P_{Y_iX_i}^H A_{Y_iX_j} P_{X_jX_j}\|_F^2\big| \\
&\leq \max\big\{\|A_{X_iX_j}\|_F^2 - \|P_{X_iX_i}^H A_{X_iX_j} P_{X_jX_j}\|_F^2, \|P_{Y_iX_i}^H A_{Y_iX_j} P_{X_jX_j}\|_F^2\big\} \\
&\leq \max\big\{(\|P_{Y_iX_i}\|_2^2 + \|P_{Y_jX_j}\|_2^2 - \|P_{Y_iX_i}\|_2^2\, \|P_{Y_jX_j}\|_2^2)\, \|A_{X_iX_j}\|_F^2, \|P_{Y_iX_i}\|_2^2\, \|A_{Y_iX_j}\|_F^2\big\} \\
&\leq \max\big\{(\|P_{Y_iX_i}\|_2^2 + \|P_{Y_jX_j}\|_2^2)\, \|A_{X_iX_j}\|_F^2, \|P_{Y_iX_i}\|_2^2\, \|A_{Y_iX_j}\|_F^2\big\} \\
&\leq \max\big\{(\|P_{Y_iX_i}\|_2^2 + \|P_{Y_jX_j}\|_2^2)\, \|A_{X_1Y_1}\|_F^2, \|P_{Y_iX_i}\|_2^2\, \|A_{X_1Y_1}\|_F^2\big\} \\
&\leq \frac{2\, \|A_{X_1Y_1}\|_F^4}{\delta^2},
\end{aligned} \tag{9}$$

where, in the first inequality, we used $|a - b| \leq \max\{a, b\}$ for $a, b \geq 0$, and Eq. (8) was applied in the second inequality. Moreover, $\|P_{X_sX_s}\|_2 \leq 1,\ s = i, j$, was used several times. In last two inequalities, the fact that $A_{X_1Y_1}$ is the off-diagonal block with the largest Frobenius norm was applied together with assumption **A2**.

Secondly,

$$\begin{aligned}
\text{Term2} &= \|P_{X_iX_i}^H A_{X_jY_j} P_{Y_jX_j}\|_F^2 + \|P_{Y_iX_i}^H A_{Y_iY_j} P_{Y_jX_j}\|_F^2 \\
&\leq \|P_{X_iX_i}\|_2^2\, \|P_{Y_jX_j}\|_2^2\, \|A_{X_jY_j}\|_F^2 + \|P_{Y_iX_i}\|_2^2\, \|P_{Y_jX_j}\|_2^2\, \|A_{Y_iY_j}\|_F^2 \\
&\leq \frac{\|A_{X_1Y_1}\|_F^4}{\delta^2} + \frac{\|A_{X_1Y_1}\|_F^6}{\delta^4} \\
&\leq \frac{2\, \|A_{X_1Y_1}\|_F^4}{\delta^2},
\end{aligned} \tag{10}$$

where, according to assumption **A1**, the bound $\|A_{X_1Y_1}\|_F^2 \leq \|\text{off}(A)\|_F^2 \leq \delta^2$ was used in the last inequality.

Next, we bound four traces in Eq. (7) using the basic properties of the CSD together with assumptions **A1** and **A2**:

$$\begin{aligned}
&|\text{Tr}_1| = \\
&= \Big|\text{Tr}\Big[\big(P_{X_iX_i}^H A_{X_iX_j} P_{X_jX_j}\big)^H \big(P_{Y_iX_i}^H A_{Y_iX_j} P_{X_jX_j} + P_{X_iX_i}^H A_{X_jY_j} P_{Y_jX_j} + P_{Y_iX_i}^H A_{Y_iY_j} P_{Y_jX_j}\big)\Big]\Big| \\
&\leq \|P_{X_iX_i}^H A_{X_iX_j} P_{X_jX_j}\|_F\, \|P_{Y_iX_i}^H A_{Y_iX_j} P_{X_jX_j} + P_{X_iX_i}^H A_{X_jY_j} P_{Y_jX_j} + P_{Y_iX_i}^H A_{Y_iY_j} P_{Y_jX_j}\|_F \\
&\leq \|P_{X_iX_i}\|_2\, \|P_{X_jX_j}\|_2\, \|A_{X_iX_j}\|_F\, \big(\|P_{Y_iX_i}\|_2\, \|P_{X_jX_j}\|_2\, \|A_{Y_iX_j}\|_F + \|P_{X_iX_i}\|_2\, \|P_{Y_jX_j}\|_2\, \|A_{X_jY_j}\|_F \\
&\qquad + \|P_{Y_iX_i}\|_2\, \|P_{Y_jX_j}\|_2\, \|A_{Y_iY_j}\|_F\big) \\
&\leq \|A_{X_iX_j}\|_F \left(\frac{2\|A_{X_1Y_1}\|_F^2}{\delta} + \frac{\|A_{X_1Y_1}\|_F^3}{\delta^2}\right) \\
&\leq \frac{3\|A_{X_1Y_1}\|_F^2}{\delta}\, \|A_{X_iX_j}\|_F,
\end{aligned} \tag{11}$$

$$
\begin{aligned}
&|\mathrm{Tr}_2| = \\
&= \left|\mathrm{Tr}\left[\left(P_{Y_iX_i}^H A_{Y_iX_j} P_{X_jX_j}\right)^H \left(P_{X_iX_i}^H A_{X_iX_j} P_{X_jX_j} + P_{X_iX_i}^H A_{X_jY_j} P_{Y_jX_j} + P_{Y_iX_i}^H A_{Y_iY_j} P_{Y_jX_j}\right)\right]\right| \\
&\leq \|P_{Y_iX_i}\|_2 \, \|P_{X_jX_j}\|_2 \, \|A_{Y_iX_j}\|_F \, \left(\|P_{X_iX_i}\|_2 \, \|P_{X_jX_j}\|_2 \, \|A_{X_iX_j}\|_F + \|P_{X_iX_i}\|_2 \, \|P_{Y_jX_j}\|_2 \, \|A_{X_jY_j}\|_F\right. \\
&\qquad \left. + \|P_{Y_iX_i}\|_2 \, \|P_{Y_jX_j}\|_2 \, \|A_{Y_iY_j}\|_F\right) \\
&\leq \|P_{Y_iX_i}\|_2 \, \|A_{Y_iX_j}\|_F \left(\|A_{X_iX_j}\|_F + \frac{\|A_{X_1Y_1}\|_F^2}{\delta} + \frac{\|A_{X_1Y_1}\|_F^3}{\delta^2}\right) \\
&\leq \frac{\|A_{X_1Y_1}\|_F^2}{\delta} \, \|A_{X_iX_j}\|_F + \frac{\|A_{X_1Y_1}\|_F^4}{\delta^2} + \frac{\|A_{X_1Y_1}\|_F^5}{\delta^3} \\
&\leq \frac{\|A_{X_1Y_1}\|_F^2}{\delta} \, \|A_{X_iX_j}\|_F + \frac{2\|A_{X_1Y_1}\|_F^4}{\delta^2},
\end{aligned}
\tag{12}
$$

$$
\begin{aligned}
&|\mathrm{Tr}_3| = \\
&= \left|\mathrm{Tr}\left[\left(P_{X_iX_i}^H A_{X_jY_j} P_{Y_jX_j}\right)^H \left(P_{X_iX_i}^H A_{X_iX_j} P_{X_jX_j} + P_{Y_iX_i}^H A_{Y_iX_j} P_{X_jX_j} + P_{Y_iX_i}^H A_{Y_iY_j} P_{Y_jX_j}\right)\right]\right| \\
&\leq \|P_{X_iX_i}\|_2 \, \|P_{Y_jX_j}\|_2 \, \|A_{X_jY_j}\|_F \, \left(\|P_{X_iX_i}\|_2 \, \|P_{X_jX_j}\|_2 \, \|A_{X_iX_j}\|_F + \|P_{Y_iX_i}\|_2 \, \|P_{X_jX_j}\|_2 \, \|A_{Y_iX_j}\|_F\right. \\
&\qquad \left. + \|P_{Y_iX_i}\|_2 \, \|P_{Y_jX_j}\|_2 \, \|A_{Y_iY_j}\|_F\right) \\
&\leq \frac{\|A_{X_1Y_1}\|_F^2}{\delta} \left(\|A_{X_iX_j}\|_F + \frac{\|A_{X_1Y_1}\|_F^2}{\delta} + \frac{\|A_{X_1Y_1}\|_F^3}{\delta^2}\right) \\
&\leq \frac{\|A_{X_1Y_1}\|_F^2}{\delta} \, \|A_{X_iX_j}\|_F + \frac{2\|A_{X_1Y_1}\|_F^4}{\delta^2},
\end{aligned}
\tag{13}
$$

$$
\begin{aligned}
&|\mathrm{Tr}_4| = \\
&= \left|\mathrm{Tr}\left[\left(P_{Y_iX_i}^H A_{Y_iY_j} P_{Y_jX_j}\right)^H \left(P_{X_iX_i}^H A_{X_iX_j} P_{X_jX_j} + P_{Y_iX_i}^H A_{Y_iX_j} P_{X_jX_j} + P_{X_iX_i}^H A_{X_jY_j} P_{Y_jX_j}\right)\right]\right| \\
&\leq \|P_{Y_iX_i}\|_2 \, \|P_{Y_jX_j}\|_2 \, \|A_{Y_iY_j}\|_F \, \left(\|P_{X_iX_i}\|_2 \, \|P_{X_jX_j}\|_2 \, \|A_{X_iX_j}\|_F + \|P_{Y_iX_i}\|_2 \, \|P_{X_jX_j}\|_2 \, \|A_{Y_iX_j}\|_F\right. \\
&\qquad \left. + \|P_{X_iX_i}\|_2 \, \|P_{Y_jX_j}\|_2 \, \|A_{X_jY_j}\|_F\right) \\
&\leq \frac{\|A_{X_1Y_1}\|_F^3}{\delta^2} \left(\|A_{X_iX_j}\|_F + \frac{\|A_{X_1Y_1}\|_F^2}{\delta} + \frac{\|A_{X_1Y_1}\|_F^2}{\delta}\right) \\
&\leq \frac{\|A_{X_1Y_1}\|_F^2}{\delta} \, \|A_{X_iX_j}\|_F + \frac{2\|A_{X_1Y_1}\|_F^4}{\delta^2}.
\end{aligned}
\tag{14}
$$

Finally, by combining the bounds from Eqs. (9)–(14), the following upper bound for the change of an arbitrary non-eliminated off-diagonal block in one parallel iteration step results:

$$
\left|\|\hat{A}_{X_iX_j}\|_F^2 - \|A_{X_iX_j}\|_F^2\right| \leq \frac{6\,\|A_{X_1Y_1}\|_F^2}{\delta}\|A_{X_iX_j}\|_F + \frac{10\,\|A_{X_1Y_1}\|_F^4}{\delta^2}. \tag{15}
$$

Remark 1. *The existence of constant δ is guaranteed by our theory developed in [3]. We can repeat here the whole discussion regarding the well-separated eigenvalues as well as clusters. This theory is valid for any parallel block-Jacobi EVD algorithm because it does not depend on a parallel ordering at all.*

Notice that in matrix notation the change of the block $A_{X_iX_j}$ can be written in the form of the two-sided orthogonal update,

$$\begin{pmatrix} \hat{A}_{X_iX_j} & \hat{A}_{X_iY_j} \\ \hat{A}_{Y_iX_j} & \hat{A}_{Y_iY_j} \end{pmatrix} = \begin{pmatrix} P_{X_iX_i} & P_{X_iY_i} \\ P_{Y_iX_i} & P_{Y_iY_i} \end{pmatrix}^H \begin{pmatrix} A_{X_iX_j} & A_{X_iY_j} \\ A_{Y_iX_j} & A_{Y_iY_j} \end{pmatrix} \begin{pmatrix} P_{X_jX_j} & P_{X_jY_j} \\ P_{Y_jX_j} & P_{Y_jY_j} \end{pmatrix}. \tag{16}$$

Here, all four blocks of A needed in the update of $A_{X_iX_j}$ are grouped together, and there are *no other* blocks involved. Hence, the off-diagonal blocks that are *not* eliminated in the parallel iteration step k can be grouped into mutually disjoint *quadruples*. Notice that for the blocking factor $w = 2p$ there are exactly $2p(2p-1)-2p = 4p(p-1)$ off-diagonal non-eliminated blocks in any parallel iteration step. These off-diagonal blocks can be split into exactly $p(p-1)$ mutually disjoint quadruples that define the *covering* of those off-diagonal blocks.

Since both transformation matrices in Eq. (16) are orthogonal, the Frobenius norm of each quadruple is *preserved* during the update. Consequently, the set of quadruples in a given iteration step represents the set of *invariants* w.r.t. the Frobenius norm. In other words, although the Frobenius norm of a given off-diagonal, non-eliminated block can change, it can change only inside its unique quadruple in such a way that the overall Frobenius norm of that quadruple remains constant. This is true for each quadruple at a given iteration step.

The covering by quadruples is defined by the GIPDO which is computed and changed at the beginning of each parallel iteration step. Hence, also the covering by quadruples changes in each iteration step and there seems to be no connection between two different coverings.

2 Asymptotic quadratic convergence

Now we prove the AQC for the parallel block-Jacobi EVD algorithm for Hermitian matrices with the GIPDO. The approach is similar to the proof of Theorem 1 in [3].

Next theorem considers the *best case scenario* when it is possible, in each parallel iteration step, to choose exactly $2p$ blocks with largest Frobenius norms for annihilation.

Theorem 1. *For the blocking factor $w = 2p$, consider one sweep (i.e., $W = w - 1$ parallel iteration steps) of the parallel block-Jacobi EVD algorithm with the GIPDO. Without loss of generality, denote the iteration steps by $k = 0, 1, \ldots, W-1$ and the off-diagonal blocks chosen by the GIPDO at step k for elimination as $A^{(k)}_{X_{k_1}Y_{k_1}}$, $A^{(k)}_{Y_{k_1}X_{k_1}}, \ldots, A^{(k)}_{X_{k_p}Y_{k_p}}$, $A^{(k)}_{Y_{k_p}X_{k_p}}$, whereby $A^{(k)}_{X_{k_1},Y_{k_1}}$ and $A^{(k)}_{Y_{k_1},X_{k_1}}$ are the off-diagonal blocks with the (equal) largest Frobenius norm. Suppose that for each k, $0 \le k \le W-1$, there exist $2kp$ smallest off-diagonal blocks that were not chosen for annihilation at the parallel iteration step k. If there exists a constant $\delta > 0$, and all matrices $P^{(k)}_{Y_{k_i}X_{k_i}}$, $1 \le i \le p$, used at iteration steps $k = 0, 1, \ldots, W-1$, satisfy $\|P^{(k)}_{Y_{k_i}X_{k_i}}\|_2 \le \|A^{(k)}_{X_{k_1}Y_{k_1}}\|_F/\delta$, then*

$$\|\mathrm{off}(A^{(W)})\|_F^2 \le \frac{25w(w-1)}{8} \left(\frac{\|\mathrm{off}(A^{(0)})\|_F^2}{\delta} \right)^2, \tag{17}$$

i.e., the parallel block-Jacobi EVD algorithm with the GIPDO converges quadratically after every sweep.

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

$$\sum_{(I,J)\in\mathcal{P}_k} \|A_{IJ}^{(k)}\|_F^2 \leq \frac{25kp}{4}\left(\frac{\|\mathrm{off}(A^{(0)})\|_F^2 - \|\mathrm{off}(A^{(k)})\|_F^2}{\delta}\right)^2. \tag{18}$$

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. (17). So it is sufficient to prove Eq. (18) instead of Eq. (17). Eq. (18) will be proved by induction. When $k = 0$, it holds trivially because both sides are zero. We assume that Eq. (18) holds for some k ($0 \leq k < W$) and show that it also holds for $k+1$.

Let us choose the $2kp$ smallest off-diagonal blocks of $A^{(k)}$ and denote their index set by $\mathcal{P}'_k$. Note that we can choose the indices in $\mathcal{P}'_k$ in a symmetric way, i.e., if $(I,J) \in \mathcal{P}'_k$ then $(J,I) \in \mathcal{P}'_k$. Then, according to the assumption, no block pair from $\mathcal{P}'_k$ was chosen for annihilation. Moreover, Eq. (18) holds also for $\mathcal{P}'_k$ (since the blocks are the smallest ones). Now, let $\mathcal{P}_{k+1} = \mathcal{P}'_k \cup \{(X_{k_1}, Y_{k_1}), (Y_{k_1}, X_{k_1}), \ldots, (X_{k_p}, Y_{k_p}), (Y_{k_p}, X_{k_p})\}$ where the blocks with indices $\{(X_{k_i}, Y_{k_i}), (Y_{k_i}, X_{k_i})\}$, $1 \leq i \leq p$, were chosen for annihilation by GIPDO at parallel iteration step k. Then $|\mathcal{P}_{k+1}| = 2(k+1)p$ and the left-hand side of Eq. (18) for off-diagonal blocks of $A^{(k+1)}$ can be computed as

$$\begin{aligned}\sum_{(I,J)\in\mathcal{P}_{k+1}} \|A_{IJ}^{(k+1)}\|_F^2 &= \sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k+1)}\|_F^2 + 2\sum_{i=1}^{p} \|A_{X_{k_i}Y_{k_i}}^{(k+1)}\|_F^2 \\ &\leq \sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k)}\|_F^2 + \sum_{(I,J)\in\mathcal{P}'_k} \left|\|A_{IJ}^{(k+1)}\|_F^2 - \|A_{IJ}^{(k)}\|_F^2\right|,\end{aligned} \tag{19}$$

since $\|A_{X_{k_i}Y_{k_i}}^{(k+1)}\|_F^2 = 0$, $1 \leq i \leq p$, and *all* off-diagonal blocks were changed.

Using Eq. (15) which estimates the change of the Frobenius norm of any off-diagonal block,

$$\begin{aligned}\sum_{(I,J)\in\mathcal{P}'_k} \left|\|A_{IJ}^{(k+1)}\|_F^2 - \|A_{IJ}^{(k)}\|_F^2\right| &\leq \frac{10\cdot 2kp\,\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^4}{\delta^2} + \frac{6\,\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^2}{\delta}\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k)}\|_F \\ &\leq \frac{20kp\,\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^4}{\delta^2} + \frac{6\,\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^2}{\delta}\sqrt{2kp}\sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k)}\|_F^2},\end{aligned}$$

where, in the second right-hand side, the Cauchy-Schwartz inequality was used. Hence, Eq. (19) can be bounded from above by the 'nearest' square,

$$\sum_{(I,J)\in\mathcal{P}_{k+1}} \|A_{IJ}^{(k+1)}\|_F^2 \leq \left(\frac{5\sqrt{kp}\,\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^2}{\delta} + \sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k)}\|_F^2}\right)^2, \tag{20}$$

since $20 < 25$ and $6\sqrt{2} < 10$.

Now recall that Eq. (18) is valid not only for $\mathcal{P}_k$ but also for $\mathcal{P}'_k$. Consequently,

$$
\begin{aligned}
\sum_{(I,J)\in\mathcal{P}_{k+1}} \|A_{IJ}^{(k+1)}\|_F^2 &\leq \left(\frac{5\sqrt{kp}\,\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^2}{\delta} + \frac{5\sqrt{kp}}{2\delta}\left(\|\mathrm{off}(A^{(0)})\|_F^2 - \|\mathrm{off}(A^{(k)})\|_F^2\right) \right)^2 \\
&= \frac{25kp}{4}\left(\frac{\|\mathrm{off}(A^{(0)})\|_F^2 - \left(\|\mathrm{off}(A^{(k)})\|_F^2 - 2\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^2\right)}{\delta} \right)^2 \\
&\leq \frac{25(k+1)p}{4}\left(\frac{\|\mathrm{off}(A^{(0)})\|_F^2 - \|\mathrm{off}(A^{(k+1)})\|_F^2}{\delta} \right)^2,
\end{aligned}
$$

where, in the last inequality, we used $k < k+1$, the lower bound

$$
\|\mathrm{off}(A^{(k)})\|_F^2 - 2\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^2 \geq \|\mathrm{off}(A^{(k)})\|_F^2 - 2\sum_{i=1}^{p}\|A_{X_{k_i}Y_{k_i}}^{(k)}\|_F^2 = \|\mathrm{off}(A^{(k+1)})\|_F^2,
$$

and the fact that the sequence of positive numbers $\{\|\mathrm{off}(A^{(k)}\|_F^2\}_{k=0}^{+\infty}$ is decreasing. The assertion follows for $k+1 = W = w-1$. □

The assumption of Theorem 1 about not choosing $2kp$ smallest off-diagonal blocks for annihilation at parallel iteration step k is, in fact, the assumption about the distribution of the off-diagonal Frobenius norm of $A^{(k)}$ in connection with its blocking. As discussed already in [2, §4.3], the GIPDO is less efficient when the off-diagonal blocks with the largest Frobenius norms lie in one block row (column), because then only one such block can be chosen for annihilation. Notice that the distribution of the off-diagonal Frobenius norm among the off-diagonal blocks can vary from one parallel iteration step to another. Consequently, in numerical experiments, one may observe the phases of the AQC interleaved with those of the slower convergence. This happens when GIPDO has to choose also off-diagonal blocks from $\mathcal{P}'_k$ for annihilation, so that $|\mathcal{P}_{k+1}| < 2(k+1)p$ and the left-hand side of Eq. (18) will not include all off-diagonal blocks for $k = W$.

For this reason, it is appropriate to analyze also the *worst case scenario* when, from $2p$ off-diagonal blocks taken for annihilation in each parallel iteration step, only 2 largest off-diagonal blocks are annihilated (notice that using the GIPDO they are *always* chosen for annihilation as first), and remaining $2p-2$ blocks are taken from the smallest blocks. As shown in the next theorem, the AQC can be proved also in this case but the length of the corresponding sweep is enlarged.

Theorem 2. *For the blocking factor $w = 2p$, consider one modified sweep V consisting of $V = \frac{w(w-1)}{2} + 1$ parallel iteration steps of the parallel block-Jacobi EVD algorithm with the GIPDO. Without loss of generality, denote the iteration steps by $k = 0, 1, \ldots, V-1$ and the off-diagonal blocks chosen by the GIPDO at step k for elimination as $A_{X_{k_1}Y_{k_1}}^{(k)}$, $A_{Y_{k_1}X_{k_1}}^{(k)}, \ldots, A_{X_{k_p}Y_{k_p}}^{(k)}$, $A_{Y_{k_p}X_{k_p}}^{(k)}$, whereby $A_{X_{k_1},Y_{k_1}}^{(k)}$ and $A_{Y_{k_1},X_{k_1}}^{(k)}$ are the off-diagonal blocks with the (equal) largest Frobenius norm. For each k, take $2p + 2(k-1)$ smallest off-diagonal blocks and assume that $2p-2$ of them were chosen for annihilation at the parallel iteration step k. If there exists a constant $\delta > 0$, and all matrices $P_{Y_{k_i}X_{k_i}}^{(k)}$, $1 \leq i \leq p$, used at iteration steps $k = 0, 1, \ldots, V-1$, satisfy*

$\|P^{(k)}_{Y_{k_i}X_{k_i}}\|_2 \leq \|A^{(k)}_{X_{k_1}Y_{k_1}}\|_F/\delta$, *then*

$$\|\mathrm{off}(A^{(V)})\|_F^2 \leq 4w^2\left(\frac{\|\mathrm{off}(A^{(0)})\|_F^2}{\delta}\right)^2, \tag{21}$$

i.e., the parallel block-Jacobi EVD algorithm with the GIPDO converges quadratically after every modified sweep.

Proof. The proof is similar to the proof of Theorem 1 with some minor adjustments. We show that for each $k = 0, 1, \ldots, V$, there exists an index set $\mathcal{P}_k = \{(I,J)|I \neq J\}$ such that $\mathcal{P}_0 = \emptyset$, $|\mathcal{P}_k| = 2p + 2(k-1)$ for $k \geq 1$, and

$$\sum_{(I,J)\in\mathcal{P}_k} \|A^{(k)}_{IJ}\|_F^2 \leq 4\left[2p + 2(k-1)\right]\left(\frac{\|\mathrm{off}(A^{(0)})\|_F^2 - \|\mathrm{off}(A^{(k)})\|_F^2}{\delta}\right)^2. \tag{22}$$

Note that when $k = V$, the left-hand side becomes $\|\mathrm{off}(A^{(V)})\|_F^2$, and the right-hand side is smaller than the right-hand side of Eq. (21). So it is sufficient to prove Eq. (22) instead of Eq. (21). Eq. (22) will be proved by induction. When $k = 0$, it holds trivially because both sides are zero. We assume that Eq. (22) holds for some k ($0 \leq k < V$) and show that it also holds for $k+1$.

Let us choose the $2p + 2(k-1)$ smallest off-diagonal blocks of $A^{(k)}$ and denote their index set by $\mathcal{P}'_k$. Note that we can choose the indices in $\mathcal{P}'_k$ in a symmetric way, i.e., if $(I,J) \in \mathcal{P}'_k$ then $(J,I) \in \mathcal{P}'_k$. Then, according to the assumption, $p-1$ block pairs from $\mathcal{P}'_k$ were chosen for annihilation. Moreover, Eq. (22) holds also for $\mathcal{P}'_k$ (since the blocks are the smallest ones). Now, let $\mathcal{P}_{k+1} = \mathcal{P}'_k \cup \{(X_{k_1}, Y_{k_1}), (Y_{k_1}, X_{k_1}), \ldots, (X_{k_p}, Y_{k_p}), (Y_{k_p}, X_{k_p})\}$ where the blocks with indices $\{(X_{k_i}, Y_{k_i}), (Y_{k_i}, X_{k_i})\}$, $1 \leq i \leq p$, were chosen for annihilation by the GIPDO at parallel iteration step k. Notice that according to the assumption only two largest blocks, (X_{k_1}, Y_{k_1}) and (Y_{k_1}, X_{k_1}), are not from $\mathcal{P}'_k$, so that $|\mathcal{P}_{k+1}| = |\mathcal{P}'_k| + 2 = 2p + 2k$. The left-hand side of Eq. (22) for off-diagonal blocks of $A^{(k+1)}$ can be computed as

$$\begin{aligned}\sum_{(I,J)\in\mathcal{P}_{k+1}} \|A^{(k+1)}_{IJ}\|_F^2 &= \sum_{(I,J)\in\mathcal{P}'_k} \|A^{(k+1)}_{IJ}\|_F^2 + 2\sum_{i=1}^{p} \|A^{(k+1)}_{X_{k_i}Y_{k_i}}\|_F^2 \\ &\leq \sum_{(I,J)\in\mathcal{P}'_k} \|A^{(k)}_{IJ}\|_F^2 + \sum_{(I,J)\in\mathcal{P}'_k} \left|\|A^{(k+1)}_{IJ}\|_F^2 - \|A^{(k)}_{IJ}\|_F^2\right|,\end{aligned} \tag{23}$$

since $\|A^{(k+1)}_{X_{k_i}Y_{k_i}}\|_F^2 = 0$, $1 \leq i \leq p$, and *all* off-diagonal blocks were changed.

Using Eq. (15) which estimates the change of the Frobenius norm of any off-diagonal block,

$$\begin{aligned}\sum_{(I,J)\in\mathcal{P}'_k} \left|\|A^{(k+1)}_{IJ}\|_F^2 - \|A^{(k)}_{IJ}\|_F^2\right| &\leq \frac{10\left[2p+2(k-1)\right]\|A^{(k)}_{X_{k_1}Y_{k_1}}\|_F^4}{\delta^2} + \frac{6\,\|A^{(k)}_{X_{k_1}Y_{k_1}}\|_F^2}{\delta} \sum_{(I,J)\in\mathcal{P}'_k} \|A^{(k)}_{IJ}\|_F \\ &\leq \frac{10\left[2p+2(k-1)\right]\|A^{(k)}_{X_{k_1}Y_{k_1}}\|_F^4}{\delta^2} + \frac{6\,\|A^{(k)}_{X_{k_1}Y_{k_1}}\|_F^2}{\delta}\sqrt{2p+2(k-1)}\sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|A^{(k)}_{IJ}\|_F^2},\end{aligned}$$

where, in the second right-hand side, the Cauchy-Schwartz inequality was used. Hence, Eq. (23) can be bounded from above by the 'nearest' square,

$$\sum_{(I,J)\in\mathcal{P}_{k+1}} \|A_{IJ}^{(k+1)}\|_F^2 \leq \left(\frac{4\sqrt{2p+2(k-1)}\,\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^2}{\delta} + \sqrt{\sum_{(I,J)\in\mathcal{P}'_k} \|A_{IJ}^{(k)}\|_F^2} \right)^2, \tag{24}$$

since $10 < 16$ and $6 < 8$.

Now recall that Eq. (22) is valid not only for $\mathcal{P}_k$ but also for $\mathcal{P}'_k$. Consequently, denoting by $\mathcal{S} \equiv \sum_{(I,J)\in\mathcal{P}_{k+1}} \|A_{IJ}^{(k+1)}\|_F^2$,

$$\begin{aligned}
\mathcal{S} \leq & \left(\frac{4\sqrt{2p+2(k-1)}\,\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^2}{\delta} + \frac{4\sqrt{2p+2(k-1)}}{2\delta}\left(\|\mathrm{off}(A^{(0)})\|_F^2 - \|\mathrm{off}(A^{(k)}\|_F^2\right) \right)^2 \\
&= 4\,[2p+2(k-1)] \left(\frac{\|\mathrm{off}(A^{(0)})\|_F^2 - \left(\|\mathrm{off}(A^{(k)}\|_F^2 - 2\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^2\right)}{\delta} \right)^2 \\
&\leq 4\,[2p+2k] \left(\frac{\|\mathrm{off}(A^{(0)}\|_F^2 - \|\mathrm{off}(A^{(k+1)}\|_F^2}{\delta} \right)^2,
\end{aligned}$$

where, in the last inequality, we used $k-1 < k$, the lower bound

$$\|\mathrm{off}(A^{(k)}\|_F^2 - 2\|A_{X_{k_1}Y_{k_1}}^{(k)}\|_F^2 \geq \|\mathrm{off}(A^{(k)}\|_F^2 - 2\sum_{i=1}^{p} \|A_{X_{k_i}Y_{k_i}}^{(k)}\|_F^2 = \|\mathrm{off}(A^{(k+1)}\|_F^2,$$

and the fact that the sequence of positive numbers $\{\|\mathrm{off}(A^{(k)}\|_F^2\}_{k=0}^{+\infty}$ is decreasing. The assertion follows for $k+1 = V = \frac{w(w-1)}{2} + 1$. □

Remark 2. *In Theorems 1 and 2, the assumption about smallest off-diagonal blocks taken for annihilation in a parallel iteration step k can be relaxed to taking an even, variable number c_k, $0 \leq c_k \leq 2p-2$, of such blocks. In that case, the length of sweep W and V is the lower and upper bound, respectively, for the number of parallel iteration steps over which the AQC will actually be observed.*

Remark 3. *In contrast to the proof of Theorem 1 in [3], all off-diagonal blocks change their Frobenius norms during one parallel iteration step under the dynamic ordering, so that there is no set of off-diagonal blocks which retain their Frobenius norms. But this fact causes no substantial difficulty, it only leads to the larger constant of order $O(w^2)$ on the right-hand side of Eqs. (17) and (21) as compared to that of order $O(w)$ in the serial algorithm–see [3].*

Remark 4. *The structure of the change of the Frobenius norm in Eq. (15) is very important for the upper bound in the form of a 'square' in Eqs. (20) and (24). Notice that powers 2 and 4 of $\|A_{X_1Y_1}^{(k)}\|_F$ together with the linear dependence on $\|A_{X_iX_j}^{(k)}\|_F$ in Eq. (15) enable to find always the upper bound in Eqs. (20) and (24) in the form of a square (albeit the constants in that square can lead to a large overestimate).*

Remark 5. *The constants* $25w(w-1)/8$ *and* $4w^2$ *seem to be much smaller than the corresponding constant in [4, Eq. (27)]. In [4],* $W' = w(w-1)/2$ *(the number of off-diagonal blocks in the upper triangle of* A*), while here* $W = w - 1$ *for the best case scenario. Hence,* $W < W'$*, and* $W = O(w)$ *while* $W' = O(w^2)$*. On the other hand, for the worst case scenario, the length of modified sweep is* $V = O(w^2)$*, i.e. of the same order as in [4]. However, new upper bounds in Eqs. (17) and (21) are both* $O(w^2)$ *for the square of the whole off-diagonal Frobenius norm, while the upper bound in [4] is* $O(w^4\sqrt{\ell})$ *for the Frobenius norm (not its square!) of one off-diagonal block where* ℓ *is the block size. Recall that* $w = 2p$*; consequently, the order estimates are also valid using the number of processors* p *instead of the blocking factor* w*.*

References

[1] M. Bečka, G. Okša, M. Vajteršic, *Dynamic ordering for a parallel block-Jacobi SVD algorithm*, Parallel Computing 28 (2002) 243-262.

[2] G. Okša, M. Vajteršic, *Efficient pre-processing in the parallel block-Jacobi SVD algorithm*, Parallel Computing 32 (2006) 166-176.

[3] G. Okša, Y. Yamamoto, M. Vajteršic, *Asymptotic quadratic convergence of the serial block-Jacobi EVD algorithm for Hermitian matrices*, 2015, submitted for publication.

[4] Y. Yamamoto, Z. Lan, S. Kudo, *Convergence analysis of the parallel classical block Jacobi method for the symmetric eigenvalue problem*, JSIAM Letters 6 (2014) 57-60.