Convergence analysis of the parallel classical block Jacobi method for the symmetric eigenvalue problem

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Abstract

We analyze convergence properties of the parallel classical block Jacobi method for the symmetric eigenvalue problem using dynamic ordering strategy of Becka et al. It is shown that the method is globally convergent. It is also shown that the order of convergence is ultimately quadratic if there are no multiple eigenvalues.

Keywords symmetric eigenvalue problem, Jacobi method, parallel computing

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1. Introduction

In this paper, we consider the problem of computing all the eigenvalues and eigenvectors of a real symmetric $n \times n$ matrix $A$. For this problem, algorithms based on tri-diagonalization of the coefficient matrix have been used as a standard procedure. However, the algorithm of tri-diagonalization has small parallel granularity and requires $O(n)$ inter-processor synchronization. Due to this, when the matrix is not very large, the overhead of synchronization becomes dominant and the performance tends to be saturated with a small number of processors.

Recently, block Jacobi methods have attracted attention as an alternative to the tri-diagonalization based approach. They are block versions of the well known Jacobi methods for the symmetric eigenvalue problem and are based on the idea of making the matrix close to diagonal by eliminating off-diagonal blocks by orthogonal transformations. Although they require more computational work than the tri-diagonalization based methods, they have desirable properties from the viewpoint of high performance computing, such as large parallel granularity and efficient use of level-3 BLAS routines [1].

There are several versions of the block Jacobi methods, which differ mainly in the order of selecting the off-diagonal blocks to be eliminated. Among them, the classical block Jacobi method, which eliminates the off-diagonal block with the largest Frobenius norm at each stage, is known for its fast convergence. Becka et al. proposed to parallelize this method using a strategy called dynamic ordering [2]. In this strategy, one selects a set of off-diagonal blocks at each stage in such a way that the sum of squares of their Frobenius norms is maximal under the constraint that they can be eliminated simultaneously, and eliminates these blocks in parallel. According to numerical experiments, this strategy has proved efficient in terms of both convergence speed and parallel efficiency. However, convergence properties of this strategy have yet to be elucidated. This is in contrast to the case of the block cyclic Jacobi method, whose convergence has been analyzed recently by Drmač [3].

In this paper, we analyze global and local convergence properties of the parallel classical block Jacobi method using dynamic ordering. In particular, we show that this method is globally convergent. We also show that the order of convergence is ultimately quadratic if there are no multiple eigenvalues. Hence, we can ensure theoretically that this method has excellent convergence properties.

This paper is structured as follows. In Section 2, we explain the parallel classical block Jacobi method with dynamic ordering. Its global and local convergence properties are discussed in Sections 3 and 4, respectively. Numerical results that support our analysis are shown in Section 5. Section 6 gives some concluding remarks.

2. The parallel classical block Jacobi method using dynamic ordering

Let $P$ be the number of processors and assume that $n$ is divisible by $2P$, though extension to a more general case is straightforward. Let $L = n/2P$ and suppose that the matrix $A^{(0)} = A$ is partitioned into blocks of size $L \times L$. We denote the $(I, J)$ block of $A$ by $A_{IJ}$. In the $k$th step of the (sequential) classical block Jacobi method, one eliminates the block $A_{XY}^{(k)}$ with the largest Frobenius norm (F-norm) by an orthogonal transformation:

$$A^{(k+1)} = (P^{(k)})^\top A^{(k)} P^{(k)}.$$  \hfill (1)

The $n \times n$ orthogonal matrix $P^{(k)}$ is defined as follows.

Let us define a $2L \times 2L$ matrix $\bar{A}^{(k)}$ by

$$\bar{A}^{(k)} = \begin{pmatrix} A_{XX}^{(k)} & A_{XY}^{(k)} \\ A_{YX}^{(k)} & A_{YY}^{(k)} \end{pmatrix}$$  \hfill (2)

and denote the eigenvector matrix of $\bar{A}^{(k)}$ by $\bar{P}^{(k)}$. Now, partition $\bar{P}^{(k)}$ into four $L \times L$ blocks $P_{XX}^{(k)}$, $P_{XY}^{(k)}$, $P_{YX}^{(k)}$, and $P_{YY}^{(k)}$.
and \( P^{(k)} \) and construct the matrix \( P^{(k)} \) by embedding these blocks into the \((X, X), (X, Y), (Y, X)\) and \((Y, Y)\) blocks of the \( n \times n \) identity matrix \( I_n \). It is easy to see that by using the \( P^{(k)} \) thus constructed, the \((X, Y)\) and \((Y, X)\) blocks of \( A^{(k+1)} \) become zero.

It is to be noted that only the \( X \)th and \( Y \)th block rows and \( X \)th and \( Y \)th block columns of \( A^{(k)} \) are updated with the transformation (1). Using this fact, one can eliminate another off-diagonal block, say \( A^{(k)}_{XY,Y} \), simultaneously with \( A^{(k)}_{XY} \) if \( X' \neq X, Y \) and \( Y' \neq X, Y \). More generally, \( P \) off-diagonal blocks, \( \{A^{(k)}_{XY,Y}\}^P_{\ell=1} \) can be eliminated in parallel if \( X_1, Y_1, \ldots, X_P, Y_P \) are all different, that is, if they are some permutation of \( 1, 2, \ldots, 2P \). In the dynamic ordering strategy of Becka et al., \( X_1, Y_1, \ldots, X_P, Y_P \) are determined under this constraint to maximize \( \sum_{\ell=1}^P \| A^{(k)}_{X_{\ell}Y_{\ell}} \|_F^2 \), where \( \| \cdot \|_F \) denotes the F-norm. Thus this method can be viewed as a generalization of the classical block Jacobi method.

The problem of finding such \( X_1, Y_1, \ldots, X_P, Y_P \) can be formulated as a maximum weight matching problem of the perfect graph of degree \( 2P \), where the edges and weights correspond to the off-diagonal blocks and their F-norms, respectively. In the implementation of Becka et al., this problem is solved approximately using a greedy algorithm, that is, by selecting the off-diagonal block with the largest F-norm first and then selecting the off-diagonal block with the largest F-norm from the not yet selected block rows and columns, and so on. In the following, we analyze the convergence of the parallel classical block Jacobi method under this greedy strategy.

3. Global convergence

We first consider the global convergence of the sequential classical block Jacobi method. Let \( w = 2P \) and \( W = w(w - 1)/2 \), the number of off-diagonal blocks in the upper triangular part. The following theorem holds.

**Theorem 1**  In the classical block Jacobi method, sum of squares of the F-norms of off-diagonal blocks satisfies the following inequality and therefore converges to zero as \( k \to \infty \).

\[
\sum_{i \neq j} \| A_{ij}^{(k+1)} \|^2_F \leq \left( 1 - \frac{1}{W} \right) \sum_{i \neq j} \| A_{ij}^{(k)} \|^2_F. \tag{3}
\]

**Proof**  This is a direct extension of the global convergence theorem for the classical Jacobi method [4] to the block case. Let us rewrite \( A^{(k)} \) and \( A^{(k+1)} \) as \( A \) and \( B \), respectively, for simplicity. Since \( A \) and \( B \) are unitarily equivalent and \( \| B_{XY} \|^2_F = \| B_{YX} \|^2_F = 0 \), it follows that

\[
\| B_{XY} \|^2_F = \| A_{XY} \|^2_F + \| A_{YX} \|^2_F + 2 \| A_{XY} \|^2_F.
\]

Noting that other diagonal blocks than \( A_{XX} \) and \( A_{YY} \) are unchanged and \( \| A \|^2_F = \| B \|^2_F \), we have

\[
\sum_{i \neq j} \| B_{ij} \|^2_F = \sum_{i \neq j} \| A_{ij} \|^2_F - 2 \| A_{XY} \|^2_F.
\]

Thus,

\[
\sum_{i \neq j} \| A_{ij} \|^2_F \leq \left( 1 - \frac{2}{w(w - 1)} \right) \sum_{i \neq j} \| A_{ij} \|^2_F.
\]

We used the fact that \( A_{XY} \) is the block with the largest F-norm in the first inequality.

(QED)

From this result, we immediately have the following theorem.

**Theorem 2**  In the parallel classical block Jacobi method with the greedy strategy, the off-diagonal elements of \( A^{(k)} \) converges to zero as \( k \to \infty \).

**Proof**  The matrices generated by the parallel greedy method also satisfy (3) because the off-diagonal block with the largest F-norm is included in the set of \( P \) blocks eliminated at the \( k \)th step. Hence, the off-diagonal blocks converge to zero as \( k \to \infty \). On the other hand, off-diagonal elements of all the diagonal blocks become zero after the first step and remain zero thereafter. This is because \( A_{XY}^{(k+1)} \) and \( A_{YY}^{(k+1)} \) become diagonal matrices for \( k = 1, 2, \ldots, P \) from the construction of the \( 2L \times 2L \) orthogonal transformations.

(QED)

This establishes global convergence of the parallel classical block Jacobi method with the greedy strategy. The eigenvectors can be computed from the product of the orthogonal matrices, as usual.

4. Local quadratic convergence

Let the eigenvalues of \( A \) be \( \lambda_1, \lambda_2, \ldots, \lambda_n \). In the following, we assume that there are no multiple eigenvalues and define \( d = \min_{i \neq j} |\lambda_i - \lambda_j| \). Before going into the analysis, we first quote the famous sin \( \Theta \) theorem [4], which will be a useful tool in our analysis.

**Theorem 3**  (sin \( \Theta \) theorem)  Let \( A \in \mathbb{R}^{n \times n} \) be a symmetric matrix and \( y \in \mathbb{R}^n \) be a vector with \( \| y \| = 1 \).

Define \( \alpha = y^T Ay \) and \( (y) = Ay - \alpha y \). Now, let \( \lambda_i \) be the eigenvalue of \( A \) that is closest to \( \alpha \), \( u_i \) be the corresponding eigenvector, \( \theta = \angle(y, u_i) \) and \( \text{gap}(\alpha) = \min_{i \neq j} |\lambda_i - \lambda_j| \). Then the following inequality holds.

\[
| \sin \theta | \leq \frac{\| (y) \|}{\text{gap}(\alpha)}.
\]

We first give a theorem on quadratic convergence of the sequential classical block Jacobi method. The scenario of the proof follows closely that of the quadratic convergence proof of the classical Jacobi method [5]. The main difference is that we need more intricate discussion using the sin \( \Theta \) theorem to bound the F-norms of the off-diagonal blocks of \( P \).

**Theorem 4**  Let \( \delta = \sum_{i \neq j} \| A_{ij}^{(m)} \|_F \). If \( wL\sqrt{W} \delta \leq d/4 \), then the matrix obtained by applying \( W \) steps of the classical block Jacobi method to \( A^{(m)} \) satisfies

\[
\| A_{ij}^{(m+W)} \|_F \leq \frac{2W^2}{d} \sqrt{E} \delta^2 \quad (I \neq J),
\]

that is, the F-norms of the off-diagonal blocks converge to zero quadratically after every \( W \) steps.

**Proof**  The proof will be given in several steps.
(i) Upper bound on \( \| A^{(m+k)} \|_F \)  The square sum of F-norms of the off-diagonal blocks at step \( m \) satisfies
\[
\sum_{j \neq i} \| A_{ij}^{(m+k)} \|_F^2 \leq 2W^2\delta^2. \tag{8}
\]
From (3), it is clear that the same bound holds for \( \sum_{j \neq i} \| A_{ij}^{(m+k)} \|_F^2 \) \( (k \geq 0) \). By taking the symmetry into account, the upper bound of \( \| A_{ij}^{(m+k)} \|_F \) is given as
\[
\| A_{ij}^{(m+k)} \|_F \leq \sqrt{W} \delta \quad (i \neq j, k \geq 0). \tag{9}
\]
(ii) Lower bound on the difference between two diagonal elements of \( A^{(m+k)} \)  Let the \( (i,j) \) element of \( A^{(k)} \) be denoted by \( a_{ij}^{(k)} \). The ith Gershgorin circle \( C_i \) of \( A^{(m+k)} \) is defined by
\[
C_i : |z - a_{ii}^{(m+k)}| \leq \sum_{j \neq i} |a_{ij}^{(m+k)}|. \tag{10}
\]
Let the number of the block to which \( i \) belongs be \( I_i \). Noting that the diagonal blocks of \( A^{(m+k)} \) are diagonal, the right hand side can be evaluated as
\[
\sum_{j \neq i} |a_{ij}^{(m+k)}| = \sum_{j \neq I_i} \sum_{j=(j-1)L+1}^{jL} |a_{ij}^{(m+k)}| \leq \sum_{j \neq I_i} \sqrt{\frac{1}{2}} \sqrt{\frac{1}{2}} \sum_{j=(j-1)L+1}^{jL} |a_{ij}^{(m+k)}|^2 \leq \sum_{j \neq I_i} \sqrt{L} \sqrt{\frac{2}{W}} \delta = \frac{w-1}{w} \cdot \frac{d}{4}, \tag{11}
\]
where we used the Cauchy-Schwarz inequality and (9). Since the radius of each circle is smaller than \( d/4 \) and the minimum distance between the eigenvalues is \( d \), each circle contains at most one eigenvalue. This means that each circle contains exactly one eigenvalue. Let the eigenvalue contained in \( C_i \) be \( \lambda_i \). Then,
\[
|a_{ii}^{(m+k)} - \lambda_i| \leq \frac{w-1}{w} \cdot \frac{d}{4} \quad (1 \leq i \leq n). \tag{12}
\]
Using the triangular inequality, we have for \( i \neq j \),
\[
|a_{ii}^{(m+k)} - a_{jj}^{(m+k)}| \geq |\lambda_i - \lambda_j| - |\lambda_i - a_{ii}^{(m+k)}| - |a_{jj}^{(m+k)} - \lambda_j| \geq d - w - \frac{d}{w} \cdot \frac{d}{4} = \frac{w + 1}{w} \cdot \frac{d}{4}. \tag{13}
\]
(iii) Change of the F-norm of an off-diagonal block by one step  Suppose that an off-diagonal block \( A_{ij}^{(m+k)} \) is changed by the elimination of \( A_{XJ}^{(m)} \). As a representative case, we consider the case of \( I = X \) and \( J \neq X, Y \). Let us rewrite \( A^{(k+m)} \) and \( A^{(k+m+1)} \) as \( A \) and \( B \), respectively, for simplicity. By denoting the eigenvector matrix of \( A \) by \( P \), we have from (1),
\[
B_{XJ} = P_{X}^T A_{XJ} + P_{Y}^T A_{YJ} \quad (J \neq X, Y). \tag{14}
\]
Hence,
\[
\| B_{XJ} \|_F \leq \| P_{X}^T \|_2 \| A_{XJ} \|_F + \| P_{Y}^T \|_2 \| A_{YJ} \|_F \leq \| A_{XJ} \|_F + \| P_{Y}^T \|_F \| A_{YJ} \|_F, \tag{15}
\]
where we used the fact that \( P_{XX} \) is a submatrix of an orthogonal matrix \( P \) and therefore \( \| P_{XX} \|_2 \leq 1 \).
Now, we evaluate \( \| P_{Y} \|_2 \). Denote the diagonal elements of \( A \) by \( a_{ii} \) \( (i = 1, 2, \ldots, 2L) \). Then, from (9) and the fact that both \( A_{XX} \) and \( A_{YY} \) are diagonal, we have the following Gershgorin circles for \( A \):
\[
\bar{C}_i : |z - a_{ii}| \leq \sqrt{LW} \delta, \tag{16}
\]
where we again used the Cauchy-Schwarz inequality to derive the right-hand side. Since \( \sqrt{LW} \delta \leq d/(4W) \) from the assumption, the radius of each circle is smaller than half of the minimum distance between diagonal elements of \( A \) given in (13). Thus all the circles are disjoint and each circle contains exactly one eigenvalue of \( A \). Let the eigenvalue of \( A \) contained in \( \bar{C} \) be \( \mu_i \), and the eigenvector corresponding to \( \mu_i \) be \( \mathbf{p}_i \).
Now, denote the ith column of the identity matrix of order \( 2L \) by \( \mathbf{e}_i \). We apply the \( \sin \Theta \) theorem by substituting \( A \) and \( \mathbf{e}_i \) into \( A \) and \( \mathbf{y} \), respectively, of the theorem. Then \( \alpha \) and \( r(\mathbf{e}_i) \) in the theorem can be calculated as
\[
\alpha_i = \mathbf{e}_i^T \mathbf{A} \mathbf{e}_i = \bar{a}_{ii}, \tag{17}
\]
\[
r(\mathbf{e}_i) = \tilde{\mathbf{A}} \mathbf{e}_i - \alpha_i \mathbf{e}_i = \tilde{a}_i - \bar{a}_i \mathbf{e}_i, \tag{18}
\]
where \( \mathbf{a}_i \) is the ith column vector of \( \tilde{\mathbf{A}} \). Thus, if \( 1 \leq i \leq L \), we have
\[
\| r(\mathbf{e}_i) \| = \sqrt{\sum_{j \neq i} \bar{a}_{jj}^2} \leq \| A_{YX} \|_F \leq \sqrt{W} \delta. \tag{19}
\]
A similar result follows in the case of \( L + 1 \leq i \leq 2L \). For gap(\( \alpha_i \)), we can derive the following lower bound:
\[
gap(\alpha_i) = \min_{\mu_j \neq \mu_i} |\mu_j - \bar{a}_{ii}| \geq \min_{\mu_j \neq \mu_i} (|\bar{a}_{ii} - \bar{a}_{jj}| - |\mu_j - \bar{a}_{jj}|) \geq \frac{w + 1}{w} \cdot \frac{d}{4} \geq \frac{d}{2}. \tag{20}
\]
By inserting (18) and (19) into (6), we have
\[
\sin \theta_i \leq \frac{\| r(\mathbf{e}_i) \|}{\text{gap}} \leq \frac{2\sqrt{W} \delta}{d}. \tag{21}
\]
where \( \theta_i = \angle (\mathbf{e}_i, \mathbf{p}_i) \). On the other hand,
\[
\sqrt{\sum_{j \neq i} \bar{p}_{ji}^2} = \sqrt{1 - \bar{p}_{ii}^2} = \sqrt{1 - (\mathbf{p}_i \cdot \mathbf{e}_i)^2} = |\sin \theta_i|. \tag{22}
\]
Combining (21) and (22), we have
\[
\| P_{YY} \|_2 \leq \sqrt{\sum_{i=1}^{L} \sum_{j=L+1}^{2L} \bar{p}_{ji}^2} \leq \sqrt{\sum_{i=1}^{L} \sum_{j \neq i} \bar{p}_{ji}^2} \leq \sum_{i=1}^{L} \sin^2 \theta_i \leq \frac{2\sqrt{W} \delta}{d}. \tag{23}
\]
Finally, insertion of (23) and (9) into (15) leads to
\[
\| A_{XJ}^{(m+k+1)} \|_F \leq \| A_{XJ}^{(m+k)} \|_F + \frac{2W \sqrt{L}}{d} \delta^2, \tag{24}
\]
which means that the F-norm of an off-diagonal block increases by at most $2W\sqrt{L}\delta^2/d$ by each elimination.

(iv) Change of the F-norm of an off-diagonal block after $W$ steps We can show by induction that among the $W$ off-diagonal blocks in the upper triangular part of $A^{(k+m)}$, there are at least $k$ blocks whose F-norm is smaller than or equal to $2W(k-1)\sqrt{L}\delta^2/d$. In fact, this proposition clearly is true for $k = 1$. Assume that it is true for some $k \geq 1$. Then we can consider two cases.

(a) If the block to be eliminated next is chosen from these $k$ blocks, it means that the F-norm of the block is smaller than or equal to $2W(k-1)\sqrt{L}\delta^2/d$. But because this is the off-diagonal block with the largest F-norm, all the off-diagonal blocks have F-norm smaller than or equal to $2W(k-1)\sqrt{L}\delta^2/d$. The F-norms of these blocks will increase by at most $2W\sqrt{L}\delta^2/d$ by the elimination. Thus, the proposition holds true also for $k + 1$.

(b) Otherwise, the F-norms of these $k$ blocks will increase by at most $2W\sqrt{L}\delta^2/d$ by the elimination. On the other hand, the F-norm of the block to be eliminated will become zero. Thus the proposition holds true for $k + 1$ also in this case.

Now that we have proved the proposition, we can put $k = W$ and readily obtain (7).

(QED)

Finally, we give a theorem on quadratic convergence of the parallel classical block Jacobi method.

Theorem 5 Under the same condition as in Theorem 4, the matrix obtained by applying $W$ steps of the parallel classical block Jacobi method to $A^{(m)}$ satisfies

$$
\|A_{jj}^{(m+W)}\|_F \leq \frac{4W^2\sqrt{L}}{d}\delta^2 \quad (I \neq J),
$$

that is, the F-norms of the off-diagonal blocks converge to zero quadratically after every $W$ steps.

Proof Steps (i) through (iii) of the proof are the same as those in the proof of Theorem 4, except that the second term in the right-hand side of (24) is replaced by $4W\sqrt{L}\delta^2/d$. This is because in the parallel algorithm, $w/2$ off-diagonal blocks are eliminated at once and therefore each off-diagonal block is updated both from the left and right. Also, it is to be noted that the $w/2$ off-diagonal blocks include the block with the largest F-norm.

As for step (iv), we consider the same proposition as in the proof of Theorem 4, where $2W(k-1)\sqrt{L}\delta^2/d$ is replaced by $4W(k-1)\sqrt{L}\delta^2/d$, and prove it by induction. We assume that the proposition is true for some $k \geq 1$ and consider two cases: (a) the block with the largest F-norm among the $w/2$ off-diagonal blocks to be eliminated next is chosen from the $k$ blocks specified in the proposition, or (b) otherwise. In either case, it can be shown with the same logic as in the proof of Theorem 4 that there are at least $k+1$ off-diagonal blocks in the upper triangular part of $A^{(k+m+1)}$ whose F-norm is smaller than or equal to $4Wk\sqrt{L}\delta^2/d$. Hence, the proposition is true also for $k + 1$. The theorem follows by putting $k = W$.

(QED)

5. Numerical results

In this section, we show an example of convergence behavior of the block Jacobi methods. As the test matrix, we use a real symmetric random matrix of order $n = 1,200$, whose elements follow the uniform distribution in $[0, 10]$. Fig. 1 shows the convergence of three types of block Jacobi methods, namely, the sequential classical block Jacobi method, parallel classical block Jacobi method, and the sequential cyclic block Jacobi method. It is clear that the convergence of both the sequential and parallel classical Jacobi methods are quadratic, as predicted by Theorems 4 and 5. The convergence of the cyclic method is also quadratic, as analyzed in [3], but the speed is slower.

6. Conclusion

In this paper, we presented theoretical convergence results for the parallel classical block Jacobi method using the dynamic ordering strategy. Our future work includes extension of the results to the case of multiple eigenvalues and evaluation of the algorithm on large-scale parallel machines.

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