Convergence of the complex Jacobi method and application to PGEP

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OUTLINE

- Complex Jacobi method
- Serial pivot orderings with permutations
- Jacobi annihilators and operators
- Positive definite generalized eigenvalue problem (PGEP)
- Cholesky-Jacobi (CJ) method for PGEP

JACOBI METHOD

- Let $\mathbf{A} \in \mathbb{C}^{n \times n}$ be Hermitian. **Jacobi method:**

$$\mathbf{A}^{(k+1)} = \mathbf{U}_k^* \mathbf{A}^{(k)} \mathbf{U}_k, \quad k \geq 0, \quad \mathbf{A}^{(0)} = \mathbf{A},$$

where $\mathbf{U}_k = R(i_k, j_k, \phi_k, \alpha_k)$ are complex plane rotations

$$R(i_k, j_k, \phi_k, \alpha_k) = \left[\begin{array}{ccccc} I & & & & \\ & \cos\phi_k & & -e^{\imath\alpha_k}\sin\phi_k & \\ & & I & & \\ & e^{-\imath\alpha_k}\sin\phi_k & & \cos\phi_k & \\ & & & & I \end{array}\right] \begin{array}{c} \\ i_k \\ \\ j_k \\ \\ \end{array}.$$

- Pair (i_k, j_k) is called **pivot pair**.

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- Pair (i_k, j_k) is called **pivot pair**.

- **Convergence:** $\mathbf{A}^{(k)} \to \mathbf{\Lambda}$, $\mathbf{\Lambda}$ diagonal matrix

- **Off-norm**: $S(\mathbf{A}) = \|\mathbf{A} - \mathrm{diag}(\mathbf{A})\|_F \to 0$

- We obtain $S(\mathbf{A}^{(k+1)}) \leq \gamma S(\mathbf{A}^{(k)}), \quad 0 < \gamma \leq 1,$

  where γ does not depend on $\mathbf{A}$.

ROTATION ANGLES

- Rotation angles α_k and ϕ_k in the kth iteration are chosen to annihilate the elements (i_k, j_k) and (j_k, i_k).

- For a fixed step k, $\alpha = \alpha_k$ and $\phi = \phi_k$ are obtained from the relation

$$\begin{bmatrix} a'_{ii} & 0 \\ 0 & a'_{jj} \end{bmatrix} = \begin{bmatrix} \cos\phi & -e^{\imath\alpha}\sin\phi \\ e^{-\imath\alpha}\sin\phi & \cos\phi \end{bmatrix}^* \begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix} \begin{bmatrix} \cos\phi & -e^{\imath\alpha}\sin\phi \\ e^{-\imath\alpha}\sin\phi & \cos\phi \end{bmatrix}.$$

- Then

$$\alpha = \arg(a_{ij})$$

and

$$\tan(2\phi) = \frac{2|a_{ij}|}{a_{ii} - a_{jj}}.$$

PIVOT ORDERINGS

- **Cyclic pivot ordering** is the sequence

$$\mathcal{O} = (i(0), j(0)), \ldots, (i(N-1), j(N-1)) \in \mathcal{O}(P_n),$$

where $N = n(n-1)/2$ and $P_n = \{(i,j) \mid 1 \leq i < j \leq n\}$.

- Visualization of an ordering $\mathcal{O}$ of P_n:

symmetric matrix of order n, $\mathrm{M}_{\mathcal{O}} = (\mathrm{m}_{rt})$,

$$\mathrm{m}_{i(k)j(k)} = \mathrm{m}_{j(k)i(k)} = k, \quad k = 0, 1, \ldots, N-1.$$

We set $\mathrm{m}_{rr} = *$, $1 \leq r \leq n$.

- Example: Serial pivot orderings, column-wise and row-wise

$$\mathrm{M}_{\mathcal{O}_c} = \begin{bmatrix} * & 0 & 1 & 3 & 6 \\ 0 & * & 2 & 4 & 7 \\ 1 & 2 & * & 5 & 8 \\ 3 & 4 & 5 & * & 9 \\ 6 & 7 & 8 & 9 & * \end{bmatrix}, \qquad \mathrm{M}_{\mathcal{O}_r} = \begin{bmatrix} * & 0 & 1 & 2 & 3 \\ 0 & * & 4 & 5 & 6 \\ 1 & 4 & * & 7 & 8 \\ 2 & 5 & 7 & * & 9 \\ 3 & 6 & 8 & 9 & * \end{bmatrix}.$$

EQUIVALENT ORDERINGS

- **Admissible transposition** on $\mathcal{O} \in \mathcal{O}(\mathcal{S})$, $\mathcal{S} \subseteq P_n$ is a transposition of two adjacent terms

$$(i_r, j_r), (i_{r+1}, j_{r+1}) \to (i_{r+1}, j_{r+1}), (i_r, j_r),$$

  provided that $\{i_r, j_r\}$ and $\{i_{r+1}, j_{r+1}\}$ are disjoint.

Two sequences $\mathcal{O}, \mathcal{O}' \in \mathcal{O}(P_n)$ are:

(i) **equivalent** (we write $\mathcal{O} \sim \mathcal{O}'$) if one can be obtained from the other by a finite set of admissible transpositions,

(ii) **shift-equivalent** ($\mathcal{O} \overset{s}{\sim} \mathcal{O}'$) if $\mathcal{O} = [\mathcal{O}_1, \mathcal{O}_2]$ and $\mathcal{O}' = [\mathcal{O}_2, \mathcal{O}_1]$, where [,] stands for concatenation,

(iii) **weak equivalent** ($\mathcal{O} \overset{w}{\sim} \mathcal{O}'$) if there exist $\mathcal{O}_i \in \mathcal{O}(P_n)$, $0 \leq i \leq r$, such that in the sequence $\mathcal{O} = \mathcal{O}_0, \mathcal{O}_1, \ldots, \mathcal{O}_r = \mathcal{O}'$ every two adjacent terms are equivalent or shift-equivalent.

CONVERGENT ORDERINGS

Theorem (Hansen 1963, Shroff and Schreiber 1989)

Methods defined by equivalent cyclic orderings generate the same matrices after each full cycle and within the same cycle they produce the same sets of orthogonal elementary matrices.

If the Jacobi method converges for some cyclic ordering, then it converges for all orderings that are weak equivalent to it.

$\rightarrow$ We enlarge the set of "convergent orderings".

INVERSE AND PERMUTATION EQUIVALENT

- Let $\mathcal{O} \in \mathcal{O}(P_n)$, $\mathcal{O} = (i_0, j_0), (i_1, j_1), \ldots, (i_{N-1}, j_{N-1})$. Then

$$\mathcal{O}^{\leftarrow} = (i_{N-1}, j_{N-1}), \ldots, (i_1, j_1), (i_0, j_0) \ \in \mathcal{O}(P_n)$$

is **inverse ordering** to $\mathcal{O}$.

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  is **inverse ordering** to $\mathcal{O}$.

- Two pivot orderings $\mathcal{O}, \mathcal{O}' \in \mathcal{O}(P_n)$ are **permutation equivalent** if

$$\mathrm{M}_{\mathcal{O}'} = \mathrm{P}\mathrm{M}_{\mathcal{O}}\mathrm{P}^T$$

  holds for some permutation matrix P. We write $\mathcal{O}' \overset{\mathrm{p}}{\sim} \mathcal{O}$.

SERIAL ORDERINGS WITH PERMUTATIONS

Examples:

$$\begin{bmatrix} * & 0 & 2 & 4 & 9 & 12 \\ 0 & * & 1 & 5 & 8 & 10 \\ 2 & 1 & * & 3 & 7 & 13 \\ 4 & 5 & 3 & * & 6 & 11 \\ 9 & 8 & 7 & 6 & * & 14 \\ 12 & 10 & 13 & 11 & 14 & * \end{bmatrix} \in \mathcal{C}_c^{(6)}, \qquad \begin{bmatrix} * & 11 & 13 & 12 & 10 & 14 \\ 10 & * & 9 & 7 & 6 & 8 \\ 11 & 9 & * & 5 & 3 & 4 \\ 12 & 6 & 5 & * & 1 & 2 \\ 13 & 7 & 3 & 1 & * & 0 \\ 14 & 8 & 4 & 2 & 0 & * \end{bmatrix} \in \mathcal{C}_r^{(6)}$$

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Formal definition:

$$\mathcal{C}_c^{(n)} = \{\mathcal{O} \in \mathcal{O}(P_n) \mid \mathcal{O} = (1,2), (\pi_3(1),3), (\pi_3(2),3), \ldots,$$

$$(\pi_n(1), n), \ldots, (\pi_n(n-1), n), \quad \pi_j \in \Pi^{(1,j-1)},\ 3 \le j \le n\},$$

$$\mathcal{C}_r^{(n)} = \{\mathcal{O} \in \mathcal{O}(P_n) \mid \mathcal{O} = (n-1, n), (n-2, \tau_{n-2}(n)), (n-2, \tau_{n-2}(n-1)), \ldots,$$

$$(1, \tau_1(n)), \ldots, (1, \tau_1(2)), \quad \tau_i \in \Pi^{(i+1,n)},\ 1 \le i \le n-2\},$$

where $\Pi^{(l_1,l_2)}$ is the set of all permutations of $\{l_1, l_1+1, \ldots, l_2\}$.

SERIAL ORDERINGS WITH PERMUTATIONS–cont.

$$\overleftarrow{\mathcal{C}}_c^{(n)} = \{\mathcal{O} \in \mathcal{O}(P_n) \mid \mathcal{O}^{\leftarrow} \in \mathcal{C}_c\},$$
$$\overleftarrow{\mathcal{C}}_r^{(n)} = \{\mathcal{O} \in \mathcal{O}(P_n) \mid \mathcal{O}^{\leftarrow} \in \mathcal{C}_r\}.$$

Examples:

$$\begin{bmatrix} * & 14 & 12 & 10 & 5 & 2 \\ 14 & * & 13 & 9 & 6 & 4 \\ 12 & 13 & * & 11 & 7 & 1 \\ 10 & 9 & 11 & * & 8 & 3 \\ 5 & 6 & 7 & 8 & * & 0 \\ 2 & 4 & 1 & 3 & 0 & * \end{bmatrix} \in \overleftarrow{\mathcal{C}}_c^{(6)}, \quad \begin{bmatrix} * & 4 & 3 & 2 & 1 & 0 \\ 4 & * & 5 & 8 & 7 & 6 \\ 3 & 5 & * & 9 & 11 & 10 \\ 2 & 8 & 9 & * & 13 & 12 \\ 1 & 7 & 11 & 13 & * & 14 \\ 0 & 6 & 10 & 12 & 14 & * \end{bmatrix} \in \overleftarrow{\mathcal{C}}_r^{(6)}$$

SERIAL ORDERINGS WITH PERMUTATIONS–cont.

$$\overleftarrow{\mathcal{C}}_c^{(n)} = \{\mathcal{O} \in \mathcal{O}(P_n) \mid \mathcal{O}^{\leftarrow} \in \mathcal{C}_c\},$$
$$\overleftarrow{\mathcal{C}}_r^{(n)} = \{\mathcal{O} \in \mathcal{O}(P_n) \mid \mathcal{O}^{\leftarrow} \in \mathcal{C}_r\}.$$

Examples:

$$\begin{bmatrix} * & 14 & 12 & 10 & 5 & 2 \\ 14 & * & 13 & 9 & 6 & 4 \\ 12 & 13 & * & 11 & 7 & 1 \\ 10 & 9 & 11 & * & 8 & 3 \\ 5 & 6 & 7 & 8 & * & 0 \\ 2 & 4 & 1 & 3 & 0 & * \end{bmatrix} \in \overleftarrow{\mathcal{C}}_c^{(6)}, \quad \begin{bmatrix} * & 4 & 3 & 2 & 1 & 0 \\ 4 & * & 5 & 8 & 7 & 6 \\ 3 & 5 & * & 9 & 11 & 10 \\ 2 & 8 & 9 & * & 13 & 12 \\ 1 & 7 & 11 & 13 & * & 14 \\ 0 & 6 & 10 & 12 & 14 & * \end{bmatrix} \in \overleftarrow{\mathcal{C}}_r^{(6)}$$

Serial orderings with permutations:

$$\mathcal{C}_{sp}^{(n)} = \mathcal{C}_c^{(n)} \cup \overleftarrow{\mathcal{C}_c}^{(n)} \cup \mathcal{C}_r^{(n)} \cup \overleftarrow{\mathcal{C}_r}^{(n)}.$$

SERIAL ORDERINGS–THEOREM

Theorem (BK, Hari)

Let $\mathcal{O} \in \mathcal{C}_{sp}^{(n)}$. Suppose that $\mathbf{A}'$ is obtained from $\mathbf{A}$ by applying one cycle of the cyclic Jacobi method defined by the ordering $\mathcal{O}$. If all rotation angles satisfy $\phi_k \in [-\frac{\pi}{4}, \frac{\pi}{4}]$, $k \geq 0$, then there is a constant γ_n depending only on n such that

$$S^2(\mathbf{A}') \leq \gamma_n S^2(\mathbf{A}), \quad 0 \leq \gamma_n < 1.$$

GENERALIZED SERIAL ORDERINGS

$$\mathcal{C}_{sg}^{(n)} = \left\{ \mathcal{O} \in \mathcal{O}(P_n) \mid \mathcal{O} \overset{\mathrm{p}}{\sim} \mathcal{O}' \overset{\mathrm{w}}{\sim} \mathcal{O}'' \text{ or } \mathcal{O} \overset{\mathrm{w}}{\sim} \mathcal{O}' \overset{\mathrm{p}}{\sim} \mathcal{O}'',\ \mathcal{O}'' \in \mathcal{C}_{sp}^{(n)} \right\}.$$

Theorem (BK, Hari)

Let $\mathcal{O} \in \mathcal{C}_{sg}^{(n)}$. Suppose that the chain connecting $\mathcal{O}$ and $\mathcal{O}'' \in \mathcal{C}_{sp}^{(n)}$ is in the canonical form and contains d shift equivalences. Let $\mathbf{A}'$ be obtained from $\mathbf{A}$ by applying $d+1$ cycles of the cyclic block Jacobi method defined by the ordering $\mathcal{O}$. If all rotation angles satisfy $\phi(k) \in [-\frac{\pi}{4}, \frac{\pi}{4}]$, $k \geq 0$, then there is a constant γ_n depending only on n such that

$$S^2(\mathbf{A}') \leq \gamma_n S^2(\mathbf{A}), \quad 0 \leq \gamma_n < 1.$$

MORE GENERAL TRANSFORMATION

- For $2 \leq i, j \leq n$ we define vectors

$$c_j = \begin{bmatrix} a_{1j} \\ \vdots \\ a_{j-1,j} \end{bmatrix}, \qquad r_i = [a_{i1}, \ldots, a_{i,i-1}],$$

  and the function

$$\text{vec} : \mathbb{C}^{n \times n} \to \mathbb{C}^{2N}, \quad N = \frac{n(n-1)}{2},$$

  such that

$$a = \text{vec}(\mathbf{A}) = [c_2^T, c_3^T, \ldots, c_n^T, r_2, r_3, \ldots, r_n]^T.$$

- Since A is Hermitian we have

$$a = \text{vec}(\mathbf{A}) = \begin{bmatrix} v \\ \bar{v} \end{bmatrix}, \quad v = [c_2^T, c_3^T, \ldots, c_n^T]^T.$$

- We define linear operator $\nu_{ij} : \mathbb{C}^{n \times n} \to \mathbb{C}^{n \times n}$ that sets the elements on positions (i, j) and (j, i) to zero.

JACOBI ANNIHILATORS

Definition

Let $\mathbf{U} = R(i,j,\phi,\alpha)$. Transformation $\mathcal{R}_{ij}(\mathbf{U})$ given with

$$\mathcal{R}_{ij}(\mathbf{U})\mathrm{vec}(\mathbf{A}) = \mathrm{vec}(\nu_{ij}(\mathbf{U}^*\mathbf{A}\mathbf{U})), \quad \mathbf{A} \in \mathbb{C}^{n\times n},$$

is called the Jacobi annihilator. As it is suggested by the notation, it depends on the matrix $\mathbf{U}$ and pair (i,j).

The class of the Jacobi annihilators $\mathcal{R}_{ij}$ is a set of all transformations

$$\mathcal{R}_{ij} = \left\{\mathcal{R}_{ij}(\mathbf{U}) \;\middle|\; \mathbf{U} = R(i,j,\phi,\alpha),\ 0 \le \phi,\alpha \le 2\pi\right\}.$$

JACOBI STEP vs. JACOBI ANNIHILATOR

Compared to the one step of the Jacobi method:

- Both processes apply a plane rotation.

- Rotation in the Jacobi method is chosen to annihilate the pivot element, while Jacobi annihilator takes an arbitrary rotation angle, and pivot element is set to zero as a result of applying operator ν_{ij}.

- Of course, these processes are different and do not produce the same matrices. Still, they share many properties.

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$\rightarrow$ Generalization of one cycle of the Jacobi method:

Definition

Let $\mathcal{O} = (i_0, j_0), (i_1, j_1), \ldots, (i_{N-1}, j_{N-1}) \in \mathcal{O}(P_n), \quad N = \frac{n(n-1)}{2}$.
Then $\mathcal{J} = \mathcal{R}_{i_{N-1}j_{N-1}} \cdots \mathcal{R}_{i_1 j_1} \mathcal{R}_{i_0 j_0}$ is a **Jacobi operator**,
for $\mathcal{R}_{i_k j_k} \in \boldsymbol{\mathcal{R}}_{i_k j_k},\ 0 \leq k \leq N-1\}$.

PGEP

- Positive definite generalized eigenvalue problem:

$$\mathbf{A}x = \lambda \mathbf{B}x, \quad x \neq 0,$$

where $\mathbf{A}, \mathbf{B} \in \mathbb{C}^{n \times n}$ are Hermitian and $\mathbf{B}$ is positive definite.

- Here we are interested in the **Jacobi methods for PGEP**.

PGEP–cont.

- Preconditioning makes diagonal entries of $\mathbf{B}$ equal to one,

$$\mathbf{A}^{(0)} = \mathbf{DAD}, \quad \mathbf{B}^{(0)} = \mathbf{DBD}, \quad \text{where } \mathbf{D} = \operatorname{diag}(b_{11}^{-\frac{1}{2}}, \ldots, b_{nn}^{-\frac{1}{2}}).$$

- Then, $\mathbf{A}^{(k+1)} = \mathbf{Z}_k^* \mathbf{A}^{(k)} \mathbf{Z}_k, \quad \mathbf{B}^{(k+1)} = \mathbf{Z}_k^* \mathbf{B}^{(k)} \mathbf{Z}_k, \quad k \geq 0,$

  where $\mathbf{Z}_k$ are nonsingular matrices that differ from the identity matrix in a 2×2 pivot block,

$$\mathbf{Z}_k = \begin{array}{cc} \begin{bmatrix} I & & & & \\ & * & & * & \\ & & I & & \\ & * & & * & \\ & & & & I \end{bmatrix} & \begin{array}{c} \\ i_k \\ \\ j_k \\ \\ \end{array} \end{array}.$$

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- **Convergence:** $\mathbf{A}^{(k)} \to \mathbf{\Lambda}$, $\mathbf{B}^{(k)} \to \mathbf{I}_n$

- **Off-norm**: $S(\mathbf{A}, \mathbf{B}) = S(\mathbf{A}) + S(\mathbf{B}) \to 0$

CHOLESKY-JACOBI method for PGEP

- Denote the pivot submatrices of $\mathbf{Z}$, $\mathbf{A}$, and $\mathbf{B}$ by $\hat{Z}$, $\hat{A}$, and $\hat{B}$, respectively.

- Submatrix $\hat{Z}$ is a product of a Cholesky factor and Jacobi rotation,
$$\hat{Z} = CJ,$$
where C and J depend on $\hat{A}$ and $\hat{B}$. Then
$$\mathbf{Z} = \begin{bmatrix} I & & & & \\ & \hat{Z}_{11} & & \hat{Z}_{12} & \\ & & I & & \\ & \hat{Z}_{21} & & \hat{Z}_{22} & \\ & & & & I \end{bmatrix}$$

- One iteration has the form
$$\mathbf{A}' = \mathbf{Z}^*\mathbf{A}\mathbf{Z}, \quad \mathbf{B}' = \mathbf{Z}^*\mathbf{B}\mathbf{Z}.$$

CJ method for PGEP–cont.

- **Choleski factor** C is obtained as $C = L^{-*}$ or $C = R^{-*}$, where
$$\begin{bmatrix} 1 & b_{ij} \\ \bar{b}_{ij} & 1 \end{bmatrix} = \hat{B} = LL^*, \quad \text{or} \quad \begin{bmatrix} 1 & b_{ij} \\ \bar{b}_{ij} & 1 \end{bmatrix} = \hat{B} = RR^*.$$
- Numerical tests (Hari 2017) show that the best accuracy properties are reached when these two approaches are combined such that we use
$$LL^* \quad \text{if } a_{ii} \leq a_{jj}, \quad \text{or} \quad RR^* \quad \text{if } a_{ii} > a_{jj}.$$
- Then we chose **Jacobi rotation** J that annihilates off-diagonal elements of
$$C^* \hat{A} C.$$
- $\hat{Z} = CJ$

CJ method for PGEP–cont.

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$$C^* \hat{A} C.$$

- $\hat{Z} = CJ$

Theorem (BK, Hari)

CJ is globally convergent under the class of generalizes serial orderings.

SUMMARY

- We proved convergence of the complex Jacobi method under a large set of so-called generalized serial orderings.
- To do that we work with a more general transformations induced by Jacobi operators. This new iterative process is not the same as the Jacobi method, but they share many properties important for the convergence proof.
- For PGEP we used Cholesky-Jacobi method and prove its convergence under generalized serial orderings.

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THANK YOU!