

On Jacobi Methods for the Positive Definite Generalized Eigenvalue Problem

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OUTLINE

- GEP and PGEP

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- Derivation of the algorithms

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- Convergence, global and asymptotic

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- Global convergence of block algorithms

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For such a pair there is a nonsingular matrix F such that

$$F^T A F = \Lambda_A, \quad F^T B F = \Lambda_B,$$

$$\Lambda_A = \text{diag}(\alpha_1, \dots, \alpha_n), \quad \Lambda_B = \text{diag}(\beta_1, \dots, \beta_n) \succ O.$$

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The **eigenpairs** of (A, B) are: $(\alpha_i/\beta_i, Fe_i)$, $1 \leq i \leq n$; $I_n = [e_1, \dots, e_n]$.

How to solve PGEP?

One can try with the transformation $(A, B) \mapsto (L^{-1}AL^{-T}, I)$, $B = LL^T$ and reduce PGEP to the standard EP for one symmetric matrix.

If L has small singular value(s), then the computed $L^{-1}AL^{-T}$ will have **corrupt eigenvalues**.

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$$(A, B) \mapsto (A_\varphi, B_\varphi) = (A \cos \varphi + B \sin \varphi, -A \sin \varphi + B \cos \varphi),$$

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We follow the second path.

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The two methods are connected: the FL method can be viewed as the HZ method with “fast scaled” transformations. So, the FL method seems to be somewhat faster and the HZ method seems to be more robust.

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When implemented as one-sided block algorithm for the GSVD, it is almost perfectly parallelizable, so parallel shared memory versions of the algorithm are highly scalable, and their speedup almost solely depends on the number of cores used.

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This property of $B^{(0)}$ is maintained during the iteration process:

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$$Z_k = \begin{bmatrix} I & & & \\ & c_k & & -s_k \\ & & I & \\ & \tilde{s}_k & & \tilde{c}_k \\ & & & & I \end{bmatrix} \begin{matrix} i(k) \\ j(k) \end{matrix}, \quad i(k) < j(k) \text{ are pivot indices at step } k,$$

$$c_k^2 + s_k^2 = \tilde{c}_k^2 + \tilde{s}_k^2 = 1 / \sqrt{1 - b_{i(k)j(k)}^2} \quad (\text{Gose 1979}).$$

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The selection of pivot pairs $(i(k), j(k))$ defines pivot strategy.

Derivation of the HZ Method

To describe step k , we assume: $A = A^{(k)}$, $A' = A^{(k+1)}$, $Z_k = Z$,

$$\hat{Z} = \begin{bmatrix} c & -s \\ \tilde{s} & \tilde{c} \end{bmatrix} \quad \text{the pivot submatrix of } Z.$$

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We have

$$A' = Z^T A Z, \quad B' = Z^T B Z \quad \left(\hat{A}' = \hat{Z}^T \hat{A} \hat{Z}, \quad \hat{B}' = \hat{Z}^T \hat{B} \hat{Z} \right).$$

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\hat{Z} is sought in the form of a product of two Jacobi rotations and one diagonal matrix. We have two possibilities:

\hat{Z} is sought in the form:

$$(a) \begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{1+b_{ij}}} & 0 \\ 0 & \frac{1}{\sqrt{1-b_{ij}}} \end{bmatrix} \begin{bmatrix} \cos(\theta - \frac{\pi}{4}) & -\sin(\theta - \frac{\pi}{4}) \\ \sin(\theta - \frac{\pi}{4}) & \cos(\theta - \frac{\pi}{4}) \end{bmatrix}$$

$$(b) \begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{1-b_{ij}}} & 0 \\ 0 & \frac{1}{\sqrt{1+b_{ij}}} \end{bmatrix} \begin{bmatrix} \cos(\theta + \frac{\pi}{4}) & -\sin(\theta + \frac{\pi}{4}) \\ \sin(\theta + \frac{\pi}{4}) & \cos(\theta + \frac{\pi}{4}) \end{bmatrix}$$

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The both possibilities yield the same algorithm.

Essential Part of the Algorithm

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$$\cos \phi = \rho \cos \theta - \xi \sin \theta$$

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$$a'_{ii} = a_{ii} + \frac{1}{1-b_{ij}^2} [(b_{ij}^2 - \sin^2 \phi) a_{ii} + 2 \cos \phi \sin \psi a_{ij} + \sin^2 \psi a_{jj}]$$

$$a'_{jj} = a_{jj} - \frac{1}{1-b_{ij}^2} [(\sin^2 \psi - b_{ij}^2) a_{jj} + 2 \cos \psi \sin \phi a_{ij} + \sin^2 \phi a_{ii}]$$

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Essential Part of the Algorithm

Let

$$b = |b_{ij}|, \quad t = \sqrt{1 - b^2}, \quad e = a_{jj} - a_{ii}, \quad \epsilon = \begin{cases} 1, & e \geq 0 \\ -1, & e < 0 \end{cases},$$

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$$u + \imath v = e^{-\imath \arg(b_{ij})} a_{ij}, \quad \tan \gamma = 2 \frac{v}{|e|}, \quad -\frac{\pi}{2} < \gamma \leq \frac{\pi}{2}$$

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Then

$$\hat{Z} = \frac{1}{\sqrt{1 - b^2}} \begin{bmatrix} \cos \phi & e^{\imath\alpha} \sin \phi \\ -e^{-\imath\beta} \sin \psi & \cos \psi \end{bmatrix}$$

Consider the Cholesky factorization of \hat{B} :

$$\begin{bmatrix} 1 & b_{ij} \\ b_{ij} & 1 \end{bmatrix} = \hat{B} = \hat{L}\hat{L}^T = \begin{bmatrix} 1 & 0 \\ a & c \end{bmatrix} \begin{bmatrix} 1 & a \\ 0 & c \end{bmatrix} = \begin{bmatrix} 1 & a \\ a & a^2 + c^2 \end{bmatrix}.$$

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$$\hat{L} = \begin{bmatrix} 1 & 0 \\ b_{ij} & \sqrt{1 - b_{ij}^2} \end{bmatrix}, \quad \hat{L}^{-1} = \begin{bmatrix} 1 & 0 \\ -\frac{b_{ij}}{\sqrt{1 - b_{ij}^2}} & \frac{1}{\sqrt{1 - b_{ij}^2}} \end{bmatrix}.$$

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$$\hat{L} = \begin{bmatrix} 1 & 0 \\ b_{ij} & \sqrt{1 - b_{ij}^2} \end{bmatrix}, \quad \hat{L}^{-1} = \begin{bmatrix} 1 & 0 \\ -\frac{b_{ij}}{\sqrt{1 - b_{ij}^2}} & \frac{1}{\sqrt{1 - b_{ij}^2}} \end{bmatrix}.$$

If we write $\hat{F}_1 = \hat{L}^{-T}$, then $\hat{F}_1^T \hat{B} \hat{F}_1 = I_2$ and

The Algorithm Based on LL^T Factorization

$$\begin{aligned}\hat{F}_1^T \hat{A} \hat{F}_1 &= \begin{bmatrix} 1 & 0 \\ f_{ij} & f_{jj} \end{bmatrix} \begin{bmatrix} a_{ii} & a_{ij} \\ a_{ij} & a_{jj} \end{bmatrix} \begin{bmatrix} 1 & f_{ij} \\ 0 & f_{jj} \end{bmatrix} \\ &= \begin{bmatrix} a_{ii} & f_{ij}a_{ii} + f_{jj}a_{ij} \\ f_{ij}a_{ii} + f_{jj}a_{ij} & f_{ij}^2 a_{ii} + 2f_{ij}f_{jj}a_{ij} + f_{jj}^2 a_{jj} \end{bmatrix} \\ &= \begin{bmatrix} a_{ii} & \frac{a_{ij} - b_{ij}a_{ii}}{\sqrt{1 - b_{ij}^2}} \\ \frac{a_{ij} - b_{ij}a_{ii}}{\sqrt{1 - b_{ij}^2}} & a_{jj} - \frac{2a_{ij} - (a_{ii} + a_{jj})b_{ij}}{1 - b_{ij}^2} b_{ij} \end{bmatrix}, \end{aligned} \quad (1)$$

where we have used $f_{ij} = -b_{ij}/\sqrt{1 - b_{ij}^2}$, $f_{jj} = 1/\sqrt{1 - b_{ij}^2}$.

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The final \hat{F} has the form $\hat{F} = \hat{F}_1 \hat{R}$, where \hat{R} is the [Jacobi transformation](#) which diagonalizes $\hat{F}_1^T \hat{A} \hat{F}_1$. Its angle ϑ is determined by the formula

The Algorithm Based on LL^T Factorization

$$\tan(2\vartheta) = \frac{2(a_{ij} - b_{ij}a_{ii})\sqrt{1 - b_{ij}^2}}{a_{ii} - a_{jj} + 2(a_{ij} - b_{ij}a_{ii})b_{ij}}, \quad -\frac{\pi}{4} \leq \vartheta \leq \frac{\pi}{4}.$$

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The transformation formulas for the diagonal elements of A read

$$a'_{ii} = a_{ii} + \tan \vartheta \cdot \frac{a_{ij} - a_{ii}b_{ij}}{\sqrt{1 - b_{ij}^2}} \quad (2)$$

$$a'_{jj} = a_{jj} - \frac{2a_{ij}b_{ij} - b_{ij}^2(a_{ii} + a_{jj})}{1 - b_{ij}^2} - \tan \vartheta \cdot \frac{a_{ij} - a_{ii}b_{ij}}{\sqrt{1 - b_{ij}^2}} \quad (3)$$

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If $a_{ii} = a_{jj}$, $a_{ij} = a_{ii}b_{ij}$ then ϑ is determined from expression $0/0$, so we choose $\vartheta = 0$. In this case a'_{ii} and a'_{jj} reduce to a_{ii} and a_{jj} , respectively.

The Algorithm Based on LL^T Factorization

This leads to a simpler matrix

$$\begin{aligned}\hat{Z} &= \frac{1}{\sqrt{1-b_{ij}^2}} \begin{bmatrix} \sqrt{1-b_{ij}^2} & -b_{ij} \\ 0 & 1 \end{bmatrix} \begin{bmatrix} c_{\vartheta} & -s_{\vartheta} \\ s_{\vartheta} & c_{\vartheta} \end{bmatrix} \\ &= \frac{1}{\sqrt{1-b_{ij}^2}} \begin{bmatrix} c_{\tilde{\vartheta}} & -s_{\tilde{\vartheta}} \\ s_{\vartheta} & c_{\vartheta} \end{bmatrix}, \quad \begin{aligned} c_{\tilde{\vartheta}} &= c_{\vartheta} \sqrt{1-b_{ij}^2} - s_{\vartheta} b_{ij}, \\ s_{\tilde{\vartheta}} &= c_{\vartheta} b_{ij} + s_{\vartheta} \sqrt{1-b_{ij}^2}. \end{aligned}\end{aligned}$$

It is easy to check that $c_{\tilde{\vartheta}}^2 + s_{\tilde{\vartheta}}^2 = 1$.

The Algorithm Based on RR^T Factorizations

Consider the RR^T factorization of \hat{B} :

$$\begin{bmatrix} 1 & b_{ij} \\ b_{ij} & 1 \end{bmatrix} = \hat{B} = \hat{R}\hat{R}^T = \begin{bmatrix} c & a \\ 0 & 1 \end{bmatrix} \begin{bmatrix} c & 0 \\ a & 1 \end{bmatrix} = \begin{bmatrix} a^2 + c^2 & a \\ a & 1 \end{bmatrix}.$$

Assuming positive c , one obtains $a = b_{ij}$, $c = \sqrt{1 - b_{ij}^2}$, hence

$$\hat{R} = \begin{bmatrix} \sqrt{1 - b_{ij}^2} & b_{ij} \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \hat{R}^{-1} = \begin{bmatrix} \frac{1}{\sqrt{1 - b_{ij}^2}} & -\frac{b_{ij}}{\sqrt{1 - b_{ij}^2}} \\ 0 & 1 \end{bmatrix}.$$

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This follows from a [result of Gose \(ZAMM 59, 1979\)](#), who found the general form of a matrix \hat{Z} which diagonalizes a positive definite symmetric matrix \hat{B} of order 2 via the congruence transformation $\hat{B} \mapsto \hat{Z}^T \hat{B} \hat{Z}$.

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If we assume $b_{11} = \dots = b_{nn}$ and the same condition for $\hat{Z}^T \hat{B} \hat{Z}$, then this form of \hat{Z} is just the [Gose's theorem](#). Later Hari generalized that result to complex matrices.

Global Convergence (Real and Complex Algorithm)

We have used the following **measure** in the convergence analysis:

$$S^2(A) = \|A - \text{diag}(A)\|_F^2, \quad S(A, B) = [S^2(A) + S^2(B)]^{1/2}.$$

The HZ method **converges globally** if

$$A^{(k)} \rightarrow \Lambda = \text{diag}(\lambda_1, \dots, \lambda_n), \quad B^{(k)} \rightarrow I_n \quad \text{as } k \rightarrow \infty,$$

holds for any initial pair of symmetric matrices (A, B) with $B \succ O$.

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We have proved the global convergence for the **serial pivot strategies**.

We are adapting the proof to hold for a new much larger class of **generalized serial strategies** which includes the class of **weak wavefront strategies**.

Asymptotic Convergence (Real and Complex Algorithm)

Let (A, B) have simple eigenvalues:

$$\lambda_1 > \lambda_2 > \cdots > \lambda_n, \quad \mu = \max\{|\lambda_1|, |\lambda_n|\},$$

$$3\delta_i = \min_{\substack{1 \leq i \leq n \\ j \neq i}} |\lambda_i - \lambda_j|, \quad 1 \leq i \leq n; \quad \delta = \min_{1 \leq i \leq n} \delta_i.$$

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Theorem

If $S(B^{(0)}) < \frac{1}{n(n-1)}$ and $S(A^{(0)}, B^{(0)}) < \frac{\delta}{2\sqrt{1+\mu^2}}$,

then for the general cyclic and for the serial strategies it holds, respectively:

$$S(A^{(N)}, B^{(N)}) \leq \sqrt{N(1+\mu^2)} \frac{S^2(A^{(0)}, B^{(0)})}{\delta}, \quad N = n(n-1)/2$$

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Multiple Eigenvalues

The situation complicates because the positive definite pair (A, B) with multiple eigenvalues, and with nearly diagonal matrices, has special structure.

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Let $A = A^*$ with $a_{11} \geq a_{22} \geq \cdots \geq a_{nn}$,
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Let

$$\lambda_1 = \dots = \lambda_{s_1} > \lambda_{s_1+1} = \dots = \lambda_{s_2} > \dots > \lambda_{s_{p-1}+1} = \dots = \lambda_{s_p},$$

where $s_p = n$.

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where $s_p = n$. Then

$$n_i = s_i - s_{i-1}, \quad 1 \leq i \leq p \quad (s_0 = 0),$$

n_i is the multiplicity of λ_{s_i} . Again, let $\mu = \max\{|\lambda_{s_1}|, |\lambda_{s_p}|\}$.

Multiple Eigenvalues

The minimum distance between two distinct eigenvalues plays special role in the analysis. Let δ_r be the **absolute gap** (separation) of λ_{s_r} from other eigenvalues,

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Then $\delta = \min_{1 \leq r \leq p} \delta_r$ is the **minimum absolute gap**.

Multiple Eigenvalues

Next we consider the following matrix block-partition

$$A = \begin{bmatrix} A_{11} & \cdots & A_{1p} \\ \vdots & \ddots & \vdots \\ A_{p1} & \cdots & A_{pp} \end{bmatrix}, \quad B = \begin{bmatrix} B_{11} & \cdots & B_{1p} \\ \vdots & \ddots & \vdots \\ B_{p1} & \cdots & B_{pp} \end{bmatrix},$$

A_{rt}, B_{rt} are $n_r \times n_t$ blocks.

For a square matrix $X = (X_{rt})$ partitioned according to n_1, \dots, n_p , let

$$\tau(X) = \|X - \text{diag}(X_{11}, \dots, X_{pp})\|_F.$$

For our positive definite pair (A, B) , let

$$\tau(A, B) = [\tau^2(A) + \tau^2(B)]^{1/2}$$

Multiple Eigenvalues

Theorem (Hari 91)

Let $D_r + E_r = A - \lambda_{s_r} B$, $\text{diag}(E_r) = 0$, $1 \leq r \leq p$. If

$$\|E_r\|_2 < \delta_r, \quad 1 \leq r \leq p,$$

then

$$\|A_{rr} - \lambda_{s_r} B_{rr}\|_F \leq \frac{1}{\delta_r} \sum_{\substack{t=1 \\ t \neq r}}^p \|A_{rt} - \lambda_{s_r} B_{rt}\|_F^2, \quad 1 \leq r \leq p$$

and

$$\sum_{s=1}^n \left| \frac{a_{ss}}{b_{ss}} - \lambda_s \right|^2 \leq \sum_{r=1}^p \|A_{rr} - \lambda_{s_r} B_{rr}\|_F^2 \leq \left[\frac{(1 + \mu^2) \tau^2(A, B)}{\delta} \right]^2.$$

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- Huge cancelations in the numerator and denominator when computing

$$\tan(2\theta) = \frac{2a_{ij} - (a_{ii} + a_{jj}) b_{ij}}{\sqrt{1 - (b_{ij})^2} (a_{ii} - a_{jj})} = \frac{\mathcal{O}(\tau^2)}{\mathcal{O}(\tau^2)}$$

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If the pivot element a_{ij} (b_{ij}) is within the diagonal block A_{rr} (B_{rr}), then we shall have:

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$$\tan(2\theta) = \frac{2a_{ij} - (a_{ii} + a_{jj}) b_{ij}}{\sqrt{1 - (b_{ij})^2} (a_{ii} - a_{jj})} = \frac{\mathcal{O}(\tau^2)}{\mathcal{O}(\tau^2)}$$

- Possibly large θ when ϵ and τ are tiny.

Multiple Eigenvalues

Let us return to the method. Let (A, B) be obtained at step k . Suppose that k is large enough, so that the last theorem holds for (A, B) . Let $\tau = \tau(A, B)$, $\epsilon = S(A, B)$. Note that $\tau \leq \epsilon$.

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This impacts asymptotic convergence and accuracy of the algorithm.

Multiple Eigenvalues

$$N = \frac{n(n-1)}{2}, \quad M = N - \sum_{r=1}^p \frac{n_r(n_r-1)}{2}, \quad n_{max} = \max_{1 \leq r \leq p} n_r$$

Let ϵ_N and τ_N denote ϵ and τ for the pair obtained after applying one sweep of the column-cyclic HZ method. If (A, B) satisfies $n \geq 3$, $p \geq 2$,

$$S(B) < \frac{1}{n(n-1)}, \quad \sqrt{1 + \mu^2} \epsilon < \min \left\{ \frac{1}{2}, \sqrt{\frac{\delta}{\mu + 1}} \right\} \delta,$$

then

- $\tau_N \leq \frac{3}{2} \sqrt{2.31^M \cdot n_{max}(1 + \mu^2)} \frac{\epsilon}{\delta} \tau$
- $\tau_N \leq \frac{3}{2} \sqrt{n_{max}(1 + \mu^2)} \frac{\epsilon^2}{\delta}$
- if $n_{max} = 2$ then $\epsilon_N \leq \frac{18}{17} \sqrt{1 + \mu^2} \frac{\epsilon^2}{\delta}$.

Goals

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- To derive a block method for PGEP
- To prove at least the global convergence of the block method

To define a block method for PGEP we start from a partition π of n

$$\pi = (n_1, n_2, \dots, n_m), \quad n_1 + n_2 + \dots + n_m = n, \quad n_i \geq 1.$$

Block-Matrix Partition

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The partition π defines block-matrix partition of any square matrix A of order n :

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1m} \\ A_{21} & A_{22} & \cdots & A_{2m} \\ \vdots & & & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mm} \end{bmatrix} \begin{matrix} n_1 \\ n_2 \\ \\ n_m \end{matrix}, \quad A_{ij} \in \mathbf{R}^{i \times j}$$

Elementary Block Matrix

Elementary block matrix \mathbf{E}_{ij} is a nonsingular $n \times n$ matrix

$$\mathbf{E}_{ij} = \begin{bmatrix} I & & & & \\ & E_{ii} & & E_{ij} & \\ & & I & & \\ & E_{ji} & & E_{jj} & \\ & & & & I \end{bmatrix} \begin{matrix} n_i \\ \\ n_j \\ \end{matrix},$$

which carries the block-matrix partition defined by π .

Block Jacobi Method for PGEP

Block Jacobi method for PGEP is iterative process of the form

$$A^{(k+1)} = F_k^T A^{(k)} F_k, \quad B^{(k+1)} = F_k^T B^{(k)} F_k, \quad k \geq 0;$$

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All matrices carry block-matrix partition defined by π : $A^{(k)} = (A_{rs}^{(k)})$,
 $B^{(k)} = (B_{rs}^{(k)})$, $F_k = (F_{rs}^{(k)})$, $k \geq 0$.

Block Jacobi Method for PGEP

At step k , the **pivot pair** (i, j) , $i < j$ is selected according to a given **pivot strategy**. Note that $i = i(k)$, $j = j(k)$.

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$n_1 = n_2 = \dots = n_m = 1 \rightarrow$ standard (element-wise) method

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Recall: element-wise methods maintained: $b_{11} = \dots = b_{nn} = 1$.

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To [simplify the algorithm](#) we need a preliminary transformation which makes both:

- transforms the diagonal elements of B to ones and
- diagonalizes all diagonal blocks of A and B .

- Set: $D^{(0)} = \text{diag}\left(\frac{1}{\sqrt{b_{11}}}, \dots, \frac{1}{\sqrt{b_{nn}}}\right)$ (i.e. $\text{diag}(D^{(0)}BD^{(0)}) = I_n$).

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- Let $D^{(0)} = \text{diag}(D_{11}^{(0)}, D_{22}^{(0)}, \dots, D_{mm}^{(0)})$ and

$$\tilde{A}_{rr} = D_{rr}^{(0)} A_{rr} D_{rr}^{(0)}, \quad \tilde{B}_{rr} = D_{rr}^{(0)} B_{rr} D_{rr}^{(0)}, \quad 1 \leq r \leq m.$$

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Apply to each pair $(\tilde{A}_{rr}, \tilde{B}_{rr})$ the HZ (or similar) method to obtain F_{rr} :

$$F_{rr}^T \tilde{A}_{rr} F_{rr} = A_{rr}^{(0)} = \text{diag}, \quad F_{rr}^T \tilde{B}_{rr} F_{rr} = I_{n_r}, \quad 1 \leq r \leq m.$$

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- **Set:** $F_0 = \text{diag}(F_{11}, F_{22}, \dots, F_{mm})$.
- **Perform:** $A^{(0)} = F_0^T D_0 A D_0 F_0, \quad B^{(0)} = F_0^T D_0 B D_0 F_0.$

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The preliminary transformation ensures that

$$(\hat{A}^{(k)}, \hat{B}^{(k)}) = \left(\begin{bmatrix} A_{ii}^{(k)} & A_{ij}^{(k)} \\ A_{ji}^{(k)} & A_{jj}^{(k)} \end{bmatrix}, \begin{bmatrix} I_{n_i} & B_{ij}^{(k)} \\ B_{ji}^{(k)} & I_{n_j} \end{bmatrix} \right), \quad k \geq 0,$$

with diagonal blocks $A_{ii}^{(k)}$ and $A_{jj}^{(k)}$. This form makes it easier to apply the element-wise HZ (or similar) algorithm which we call here the [kernel algorithm](#).

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For the complete description of the block HZ method one has to specify the **pivot strategy** and the **stopping criterion**.

For the latter, one can try with $S(A, B) \leq \|A\|_F \epsilon$ or with $S(A_S, B) \leq \epsilon$ where $A_S = \Delta A \Delta$ with diagonal Δ which makes $\text{diag}(|A_S|) = I_n$.

However, these are yet open problems as are all those concerning the global and asymptotic convergence and high relative accuracy.

THANK YOU.

Estação Neumayer III
21.02.2016 - 04:50h

Edit Enael Pires

