The Complex Cholesky-Jacobi Algorithm for PGEP

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- GEP, PGEP

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- Stability and High Relative Accuracy (HRA)

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The eigenpairs of (A, B) are: $(\alpha_i/\beta_i, Fe_i), \ 1 \leq i \leq n$,

here $I_n = [e_1, \ldots, e_n]$

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To detect whether B is well-behaved, it is sufficient to check whether

$$\kappa_2(B_S), \quad B_S = [\mathrm{diag}(B)]^{-1/2} B [\mathrm{diag}(B)]^{-1/2} \quad \text{is small.}$$

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Hence, probably the best choice for the kernel algorithm are element-wise diagonalization methods.

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- Two sided methods can smoothly, timely and cost effectively stop the process.

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We have recently derived their "equally promising" complex counterparts.

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Derivation of the Complex CJ Method

Starting with a positive definite pair (A, B), CJ first makes unit diagonal in B:

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Here each F_k is elementary plane matrix defined by the *pivot pair* $(i(k), j(k))$ and the *pivot submatrix* $\hat{F}_k$

$$F_k = \begin{array}{cl} \left[\begin{array}{ccccc} I & & & & \\ & * & & * & \\ & & I & & \\ & * & & * & \\ & & & & I \end{array}\right] & \begin{array}{l} \\ i(k) \\ \\ j(k) \\ \\ \end{array} \end{array}, \qquad \hat{F}_k = \begin{bmatrix} * & * \\ * & * \end{bmatrix}$$

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Then we have

$$A' = F^* A F, \quad B' = F^* B F \qquad \left(\hat{A}' = \hat{F}^* \hat{A} \hat{F}, \quad \hat{B}' = \hat{F}^* \hat{B} \hat{F}\right).$$

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The goal is to compute $\hat{F}$ that diagonalizes $\hat{A}$ and reduces $\hat{B}$ to I_2.

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It chooses the algorithm which is for the given data (that is $(\hat{A}, \hat{B})$)

more accurate.

The Derivation of the LL^*J Algorithm

Consider the Cholesky foctorization of $\hat{B}$: $\hat{B} = \hat{L}\hat{L}^*$,

$$\begin{bmatrix} 1 & b_{ij} \\ \bar{b}_{ij} & 1 \end{bmatrix} = \hat{B} = \hat{L}\hat{L}^* = \begin{bmatrix} 1 & 0 \\ \bar{a} & \bar{c} \end{bmatrix} \begin{bmatrix} 1 & a \\ 0 & c \end{bmatrix} = \begin{bmatrix} 1 & a \\ \bar{a} & |a|^2 + |c|^2 \end{bmatrix}$$

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$$\hat{L} = \begin{bmatrix} 1 & 0 \\ \bar{b}_{ij} & \tau \end{bmatrix}, \qquad \hat{L}^{-1} = \frac{1}{\tau} \begin{bmatrix} \tau & 0 \\ -\bar{b}_{ij} & 1 \end{bmatrix}, \qquad \hat{L}^{-*} = \frac{1}{\tau} \begin{bmatrix} \tau & -b_{ij} \\ 0 & 1 \end{bmatrix}.$$

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Let $\hat{F}_1 = \hat{L}^{-*}$. Then $\hat{F}_1^* \hat{B} \hat{F}_1 = I_2$ and

$$\hat{F}_1^* \hat{A} \hat{F}_1 = \begin{bmatrix} a_{ii} & (a_{ij} - b_{ij} a_{ii})/\tau \\ (\bar{a}_{ij} - \bar{b}_{ij} a_{ii})/\tau & a_{jj} - \frac{a_{ij}\bar{b}_{ij} + \bar{a}_{ij} b_{ij} - (a_{ii} + a_{jj})|b_{ij}|^2}{1 - |b_{ij}|^2} \end{bmatrix}.$$

The Derivation of the LL^*J Algorithm

The final $\hat{F}$ is obtained as product $\hat{F} = \hat{F}_1 \hat{R}_1$ where

$\hat{R}_1$ is the complex Jacobi rotation which diagonalizes $\hat{F}_1^* \hat{A} \hat{F}_1$.

Let us assume

$$\hat{R}_1 = \begin{bmatrix} c_{\vartheta_1} & -s_{\vartheta_1}^{+} \\ s_{\vartheta_1}^{-} & c_{\vartheta_1} \end{bmatrix}, \qquad c_{\vartheta_1} = \cos\vartheta_1, \qquad s_{\vartheta_1}^{\pm} = e^{\pm\imath\epsilon_1} \sin\vartheta_1.$$

Then the angles ϑ_1 and ϵ_1 are determined by the formulas

$$\begin{aligned} \epsilon_1 &= \arg(a_{ij} - b_{ij} a_{ii}), \\ \tan(2\vartheta_1) &= \frac{2|a_{ij} - a_{ii} b_{ij}| \sqrt{1 - |b_{ij}|^2}}{a_{ii} - a_{jj} + a_{ij}\bar{b}_{ij} + \bar{a}_{ij} b_{ij} - 2a_{ii}|b_{ij}|^2}, \quad -\frac{\pi}{4} \le \vartheta_1 \le \frac{\pi}{4}. \end{aligned}$$

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The transformation formulas for the diagonal elements of A read

$$\begin{aligned}
a'_{ii} &= a_{ii} + \tan\vartheta_1 \cdot \frac{|a_{ij} - a_{ii}b_{ij}|}{\sqrt{1-|b_{ij}|^2}}, \\
a'_{jj} &= a_{jj} - \frac{a_{ij}\bar{b}_{ij} + \bar{a}_{ij}b_{ij} - (a_{ii}+a_{jj})|b_{ij}|^2}{1-|b_{ij}|^2} - \tan\vartheta_1 \cdot \frac{|a_{ij} - a_{ii}b_{ij}|}{\sqrt{1-|b_{ij}|^2}}.
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In the case $a_{ii} = a_{jj}$, $a_{ij} = a_{ii} b_{ij}$, $\tan(2\vartheta_1)$ has the form $0/0$.

The Derivation of the LL^*J Algorithm

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In the case $a_{ii} = a_{jj}$, $a_{ij} = a_{ii} b_{ij}$, $\tan(2\vartheta_1)$ has the form $0/0$.

Then we choose $\vartheta_1 = 0$, so that $a'_{ii} = a_{ii}$ and $a'_{jj} = a_{jj}$.

The Derivation of the LL^*J Algorithm

$$
\begin{aligned}
\hat{F} &= \frac{1}{\sqrt{1-|b_{ij}|^2}} \begin{bmatrix} \sqrt{1-|b_{ij}|^2} & -b_{ij} \\ 0 & 1 \end{bmatrix} \begin{bmatrix} c_{\vartheta_1} & -s_{\vartheta_1}^{+} \\ s_{\vartheta_1}^{-} & c_{\vartheta_1} \end{bmatrix} \\
&= \frac{1}{\sqrt{1-|b_{ij}|^2}} \begin{bmatrix} c_{\tilde{\vartheta}_1} & -s_{\tilde{\vartheta}_1} \\ s_{\vartheta_1}^{-} & c_{\vartheta_1} \end{bmatrix} = \begin{bmatrix} c1 & -s1 \\ s2 & c2 \end{bmatrix},
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This algorithm works well, but we can still reduce the number of floating point operations per iteration step. This is accomplished by transforming the complex element $c1$ into $|c1|$.

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$$\hat{F} = \begin{bmatrix} c1 & -s1 \\ s2 & c2 \end{bmatrix}, \quad \begin{array}{ll} c1 = c_{\vartheta_1} - s_{\vartheta_1}^- b_{ij}/\sqrt{1-|b_{ij}|^2}, & c2 = c_{\vartheta_1}/\sqrt{1-|b_{ij}|^2} \\ s1 = c_{\vartheta_1} b_{ij}/\sqrt{1-|b_{ij}|^2} + s_{\vartheta_1}^+, & s2 = s_{\vartheta_1}^-/\sqrt{1-|b_{ij}|^2} \end{array}$$

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The obtained algorithm we call LL^*J algorithm.

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$$\hat{R} = \begin{bmatrix} \tau & b_{ij} \\ 0 & 1 \end{bmatrix}, \qquad \hat{R}^{-1} = \frac{1}{\tau} \begin{bmatrix} 1 & -b_{ij} \\ 0 & \tau \end{bmatrix}, \qquad \hat{R}^{-*} = \frac{1}{\tau} \begin{bmatrix} 1 & 0 \\ -\bar{b}_{ij} & \tau \end{bmatrix}.$$

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If we write $\hat{F}_2 = \hat{R}^{-*}$, then $\hat{F}_2^* \hat{B} \hat{F}_2 = \hat{R}^{-1} \hat{B} \hat{R}^{-*} = I_2$ and we have

The Derivation of the RR^*J Algorithm

$$\hat{F}_2^* \hat{A} \hat{F}_2 = \begin{bmatrix} a_{ii} - \frac{a_{ij}\bar{b}_{ij} + \bar{a}_{ij} b_{ij} - (a_{ii}+a_{jj})|b_{ij}|^2}{\tau^2} & (a_{ij} - a_{jj} b_{ij})/\tau \\ (\bar{a}_{ij} - a_{jj}\bar{b}_{ij})/\tau & a_{jj} \end{bmatrix}.$$

The Derivation of the RR^*J Algorithm

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Then the parameters ϵ_2 and ϑ_2 are determined by the formulas

$$\begin{aligned} \epsilon_2 &= \arg(a_{ij} - b_{ij} a_{jj}), \\ \tan(2\vartheta_2) &= \frac{2|a_{ij} - a_{jj} b_{ij}| \sqrt{1 - |b_{ij}|^2}}{a_{ii} - a_{jj} - (a_{ij}\bar{b}_{ij} + \bar{a}_{ij} b_{ij}) + 2a_{jj}|b_{ij}|^2}, \quad -\frac{\pi}{4} \le \vartheta_2 \le \frac{\pi}{4}. \end{aligned}$$

The Derivation of the RR^*J Algorithm

The transformation formulas for the diagonal elements of A:

$$
\begin{aligned}
a'_{ii} &= a_{ii} - \frac{a_{ij}\bar{b}_{ij} + \bar{a}_{ij}b_{ij} - (a_{ii}+a_{jj})|b_{ij}|^2}{1-|b_{ij}|^2} + \tan\vartheta_2 \cdot \frac{|a_{ij} - a_{jj}b_{ij}|}{\sqrt{1-|b_{ij}|^2}}, \\
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In that case a'_{ii} and a'_{jj} reduce to a_{ii} and a_{jj}, respectively.

The Derivation of the RR^*J Algorithm

Let $c_{\vartheta_2} = \cos\vartheta_2$, $s^{\pm}_{\vartheta_2} = e^{\pm\imath\epsilon_2}\sin\vartheta_2$. Then

$$
\begin{aligned}
\hat{F} &= \frac{1}{\sqrt{1-|b_{ij}|^2}} \left[\begin{array}{cc} 1 & 0 \\ -\bar{b}_{ij} & \sqrt{1-|b_{ij}|^2} \end{array}\right] \left[\begin{array}{cc} c_{\vartheta_2} & -s^{+}_{\vartheta_2} \\ s^{-}_{\vartheta_2} & c_{\vartheta_2} \end{array}\right] \\
&= \frac{1}{\sqrt{1-|b_{ij}|^2}} \left[\begin{array}{cc} c_{\vartheta_2} & -s^{+}_{\vartheta_2} \\ s_{\tilde{\vartheta}_2} & c_{\tilde{\vartheta}_2} \end{array}\right] = \left[\begin{array}{cc} c1 & -s1 \\ s2 & c2 \end{array}\right],
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$$

$$
\begin{aligned}
c1 &= c_{\vartheta_2}/\sqrt{1-|b_{ij}|^2}, \qquad c2 = c_{\vartheta_2} + s^{+}_{\vartheta_2}\bar{b}_{ij}/\sqrt{1-|b_{ij}|^2}, \\
s1 &= s^{+}_{\vartheta_2}/\sqrt{1-|b_{ij}|^2}^{\,+}, \qquad s2 = s^{-}_{\vartheta_2} - c_{\vartheta_2}\bar{b}_{ij}/\sqrt{1-|b_{ij}|^2}.
\end{aligned}
$$

We can postmultiply $\hat{F}$ by $\mathrm{diag}(1\,,\, \bar{c}_{\tilde{\vartheta}_2}/|c_{\tilde{\vartheta}_2}|)$ provided that $c_{\tilde{\vartheta}_2} \neq 0$. This ensures that (the updated) $\hat{F}$ has nonnegative diagonal elements.

The Complex Cholesky-Jacobi Method

The CJ method can briefly be defined as follows:

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Only the above definition warrants the HRA of the algorithm and it is in complete agreement with the behavior of the real *CJ* method.

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- It requires B to be positive definite (it solves PGEP)

Theorem

Let $A = A^* \succ O$, $B = B^* \succ O$ *and* $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, $\lambda_i \in \sigma(A, B)$.
Let $A_S = D_A^{-1/2} A D_A^{-1/2}$, $B_S = D_B^{-1/2} B D_B^{-1/2}$, $D_A = diag(A)$, $D_B = diag(B)$

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Let δA, δB *be Hermitian perturbations and* $\tilde{\lambda}_1 \geq \tilde{\lambda}_2 \geq \cdots \geq \tilde{\lambda}_n$ *the eigenvalues of* $(A + \delta A, B + \delta B)$.

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If

$$\varepsilon_{A_S} \kappa_2(A_S) < 1 \quad \text{and} \quad \varepsilon_{B_S} \kappa_2(B_S) < 1,$$

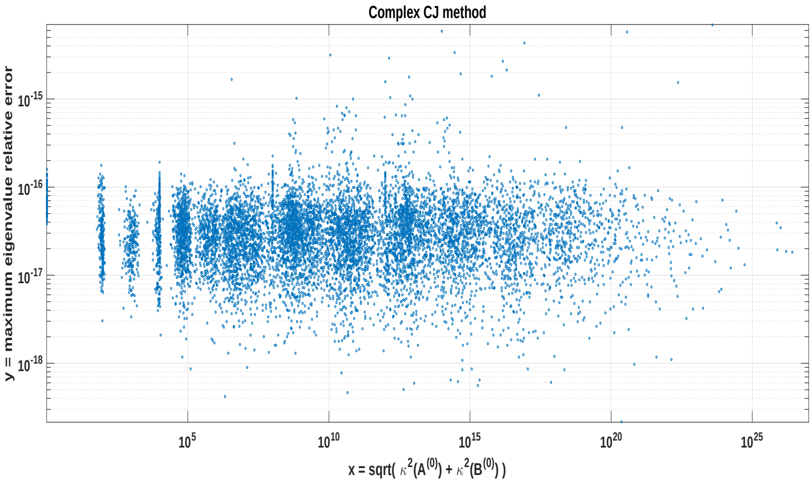
then

$$\max_{1 \leq i \leq n} \frac{|\tilde{\lambda}_i - \lambda_i|}{\lambda_i} \leq \frac{\varepsilon_{A_S} \kappa_2(A_S) + \varepsilon_{B_S} \kappa_2(B_S)}{1 - \varepsilon_{B_S} \kappa_2(B_S)} \leq \frac{\sqrt{\kappa_2(A_S)^2 + \kappa_2(B_S)^2} \sqrt{\varepsilon_{A_S}^2 + \varepsilon_{B_S}^2}}{1 - \varepsilon_{B_S} \kappa_2(B_S)}.$$

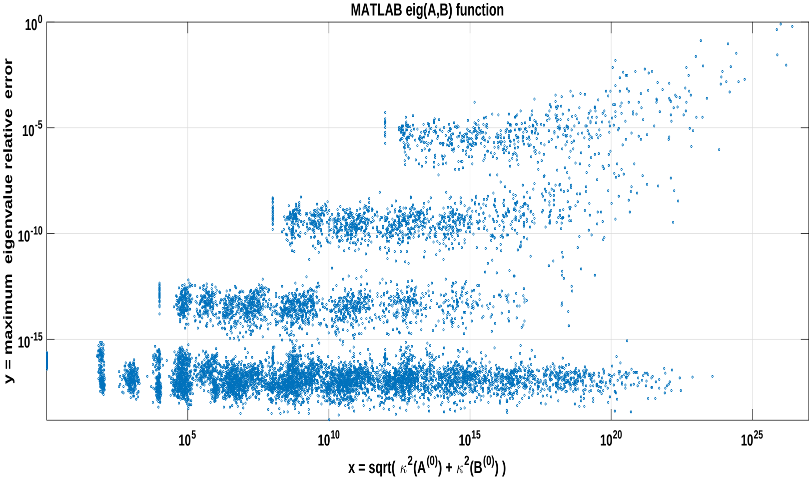
Relative Accuracy

$$
\begin{aligned}
\varrho_{(A,B)} &= \max_{1\le i\le n} \frac{|\tilde{\lambda}_i - \lambda_i|}{\lambda_i} \Big/ \sqrt{\kappa_2^2(A_S) + \kappa_2^2(B_S)} \\
\chi_{(A,B)} &= \sqrt{\kappa_2^2(A^{(0)}) + \kappa_2^2(B^{(0)})} \\
\mathcal{E} &= \{(\chi_{(A,B)}\ ,\ \varrho_{(A,B)}) :\ (A,B) \in \Upsilon\}.
\end{aligned}
$$

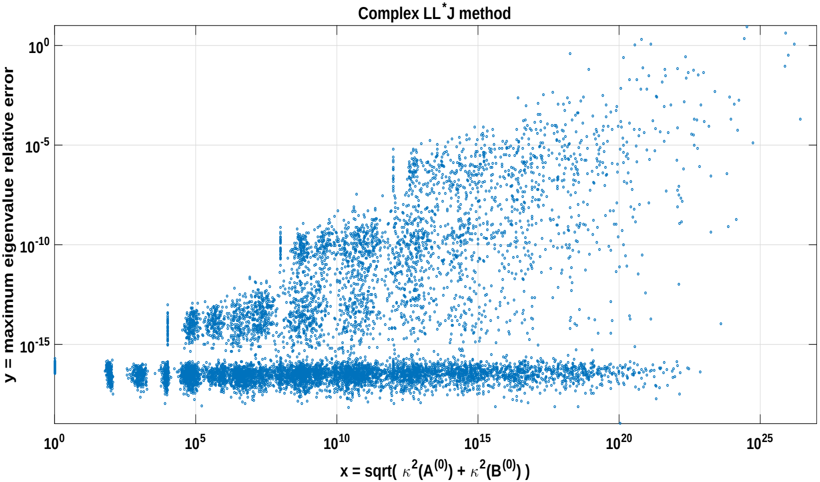
Relative Errors: *CJ* vs. MATLAB eig(A,B)



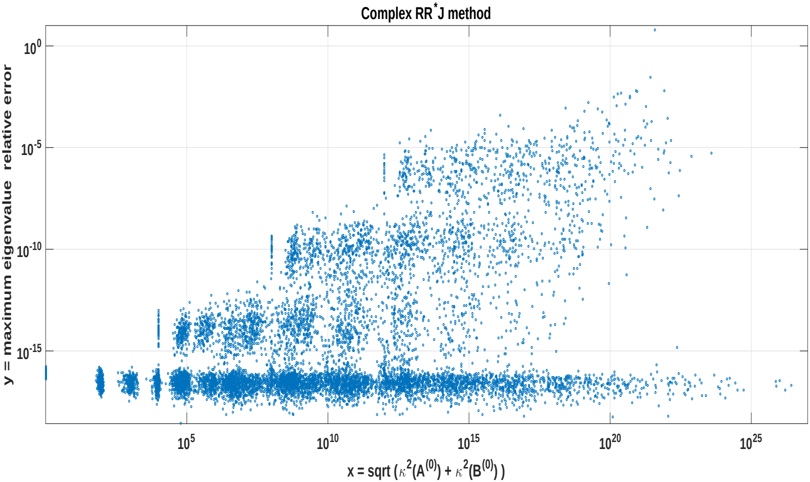
Relative Errors: *CJ* vs. MATLAB eig(A,B)



Relative Errors: $LL * J$



Relative Errors: $RR * J$



Relative Errors: Opposite Choice Than in *CJ*