On Jacobi Methods for the Positive Definite Generalized Eigenvalue Problem

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- GEP and PGEP

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- Derivation of the algorithms

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- We are considering element-wise, two-sided Jacobi-type methods for PGEP which can be used as kernel algorithms for the block methods.

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

$$F^T AF = \Lambda_A\,, \qquad F^T BF = \Lambda_B,$$

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

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

Little Proof

$$
\begin{aligned}
F^T A F = \Lambda_A \quad &\Rightarrow \quad AF = F^{-T}\Lambda_A, \\
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$$A\,Fe_i = BF\,\mathrm{diag}(\alpha_1/\beta_1, \ldots, \alpha_n/\beta_n)e_i = (\alpha_i/\beta_i)\,B\,Fe_i, \quad 1 \le i \le n.$$

$\square$

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.
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Then one can try to maximize the minimum eigenvalue of B by rotating the pair

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

or derive a method which works with the initial pair (A, B).

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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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(In this paper the method was first time referred to as the HZ method!)

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

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

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

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

To describe step k, we assume:

$$A = A^{(k)}, \quad A' = A^{(k+1)}, \quad Z_k = Z,$$

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

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

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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:

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

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

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The both possibilities yield the same algorithm.

Essential Part of the Algorithm

$$\xi = \frac{b_{ij}}{\sqrt{1+b_{ij}}+\sqrt{1-b_{ij}}}, \quad \rho = \xi + \sqrt{1-b_{ij}}, \quad \xi^2+\rho^2=1,$$

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$$\begin{aligned}
\cos\phi &= \rho\cos\theta - \xi\sin\theta \\
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$$\begin{aligned}
a'_{ii} &= a_{ii} + \frac{1}{1-b_{ij}^2}\left[(b_{ij}^2 - \sin^2\phi)\, a_{ii} + 2\cos\phi\sin\psi\, a_{ij} + \sin^2\psi\, a_{jj}\right] \\
a'_{jj} &= a_{jj} - \frac{1}{1-b_{ij}^2}\left[(\sin^2\psi - b_{ij}^2)\, a_{jj} + 2\cos\psi\sin\phi\, a_{ij} + \sin^2\phi\, a_{ii}\right]
\end{aligned}$$

There are more formulas!

$$\rho = \frac{1}{2}(\sqrt{1+b_{ij}} + \sqrt{1-b_{ij}}), \quad 2\rho\xi = b_{ij}.$$

It is easy to show the following relations: $\quad |\xi| \leq \sqrt{2}/2$, $\sqrt{2}/2 \leq \rho \leq 1$.

$$\begin{aligned}
\cos\phi\sin\psi &= \cos\theta\sin\theta - \rho\xi = 0.5\,(\sin 2\theta - b_{ij}), \\
\cos\psi\sin\phi &= \cos\theta\sin\theta + \rho\xi = 0.5\,(\sin 2\theta + b_{ij}), \\
\cos\phi\cos\psi &= \rho^2\cos^2\theta - \xi^2\sin^2\theta, \\
\sin\phi\sin\psi &= \rho^2\sin^2\theta - \xi^2\cos^2\theta.
\end{aligned}$$

$$\begin{aligned}
\min\{\cos\phi\,,\,\cos\psi\} &\geq \rho\cos\theta - \frac{|b_{ij}|}{2\rho}|\sin\theta| \geq (\rho - \frac{|b_{ij}|}{2\rho})\cos\theta > 0, \\
\max\{\cos\phi\,,\,\cos\psi\} &= \rho\cos\theta + |\xi\sin\theta| \geq \cos(\theta) \geq \frac{\sqrt{2}}{2}.
\end{aligned}$$

There are more formulas!

Let $\sin\gamma = b_{ij}$, $\cos\gamma = \sqrt{1-b_{ij}^2}$. Then

$$\frac{1}{\cos\gamma}\begin{bmatrix} a_{ii} & a_{ij} \\ a_{ij} & a_{jj} \end{bmatrix}\begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\psi & \cos\psi \end{bmatrix} = \begin{bmatrix} \cos\psi & -\sin\psi \\ \sin\phi & \cos\phi \end{bmatrix}\begin{bmatrix} a'_{ii} & \\ & a'_{jj} \end{bmatrix},$$

$$\frac{1}{\cos\gamma}\begin{bmatrix} 1 & b_{ij} \\ b_{ij} & 1 \end{bmatrix}\begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\psi & \cos\psi \end{bmatrix} = \begin{bmatrix} \cos\psi & -\sin\psi \\ \sin\phi & \cos\phi \end{bmatrix},$$

$$\begin{aligned} \cos\gamma &= \frac{\cos\phi}{\cos\psi} + b_{ij}\tan\psi = \frac{\cos\psi}{\cos\phi} - b_{ij}\tan\phi, \\ 2\cos(\phi+\psi)a_{ij} &= a_{ii}\sin(2\phi) - a_{jj}\sin(2\psi). \end{aligned}$$

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$$
\begin{aligned}
a'_{ii} &= \frac{1}{\cos\gamma}\left(a_{ii}\frac{\cos\phi}{\cos\psi} + a_{ij}\tan\psi\right) = \frac{a_{ii} + a_{ij}\frac{\sin\psi}{\cos\phi}}{1 + b_{ij}\frac{\sin\psi}{\cos\phi}}, \\
a'_{jj} &= \frac{1}{\cos\gamma}\left(a_{jj}\frac{\cos\psi}{\cos\phi} - a_{ij}\tan\phi\right) = \frac{a_{jj} - a_{ij}\frac{\sin\phi}{\cos\psi}}{1 - b_{ij}\frac{\sin\phi}{\cos\psi}}.
\end{aligned}
$$

We also have

$$
\phi + \psi = 2\theta\,, \qquad \text{hence} \qquad \begin{aligned} \phi &= \theta + \gamma/2, \\ \psi &= \theta - \gamma/2. \end{aligned}
$$

All these relations are used in the global convergence proof and in the proof of high relative accracy of the method.

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It is proved that that pivot submatrix of Z has form

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Digression: Complex Matrices

If $A = A^*$ and $B = B^*$ are complex, with $B \succ O$ and $\mathrm{diag}(B) = I_n$, then one step of the HZ method uses the transformation

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We obtain $\hat{A}' = \hat{Z}^* \hat{A} \hat{Z}, \quad \hat{B}' = \hat{Z}^* \hat{B} \hat{Z}$. $\hat{Z}$ is sought as product of two complex Jacobi rotations and two diagonal matrices.

$\hat{Z}$ is sought in the form:

$$
\begin{array}{ccc}
 & \hat{B} \to \mathrm{diag} & \hat{B} \to I_2 \\
 & \uparrow & \uparrow
\end{array}
$$

$$
\hat{Z} = \begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} e^{\imath \arg(b_{ij})} \\ \frac{\sqrt{2}}{2} e^{-\imath \arg(b_{ij})} & \frac{\sqrt{2}}{2} \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{\sqrt{1+|b_{ij}|}} & 0 \\ 0 & \frac{1}{\sqrt{1-|b_{ij}|}} \end{bmatrix}
$$

$$
\cdot \begin{bmatrix} \cos(\theta + \frac{\pi}{4}) & e^{\imath\alpha} \sin(\theta + \frac{\pi}{4}) \\ -e^{-\imath\alpha} \sin(\theta + \frac{\pi}{4}) & \cos(\theta + \frac{\pi}{4}) \end{bmatrix} \cdot \begin{bmatrix} e^{\imath\omega_i} & 0 \\ 0 & e^{\imath\omega_j} \end{bmatrix}
$$

$$
\begin{array}{cc}
\downarrow & \downarrow \\
\hat{A} \to \mathrm{diag} & \mathrm{diag}(\hat{Z}) \succ O
\end{array}
$$

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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$$\begin{aligned}
u + \imath\, v &= e^{-\imath \arg(b_{ij})}\, a_{ij}, \qquad \tan\gamma = 2\tfrac{v}{|e|}, \quad -\tfrac{\pi}{2} < \gamma \leq \tfrac{\pi}{2} \\
\tan 2\theta &= \epsilon \frac{2u-(a_{ii}+a_{jj})b}{t\sqrt{e^2+4v^2}}, \quad -\tfrac{\pi}{4} < \theta \leq \tfrac{\pi}{4} \\
2\cos^2\phi &= 1 + b\sin 2\theta + t\cos 2\theta\cos\gamma, \qquad 0 \leq \phi \leq \tfrac{\pi}{2} \\
2\cos^2\psi &= 1 - b\sin 2\theta + t\cos 2\theta\cos\gamma, \qquad 0 \leq \psi \leq \tfrac{\pi}{2} \\
e^{\imath\alpha}\sin\phi &= \frac{e^{\imath \arg(b_{ij})}}{2\cos\psi}\left[\sin 2\theta - b - \imath t\cos 2\theta\sin\gamma\right] \\
e^{-\imath\beta}\sin\psi &= \frac{e^{-\imath \arg(b_{ij})}}{2\cos\phi}\left[\sin 2\theta + b + \imath t\cos 2\theta\sin\gamma\right].
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\end{aligned}$$

Then

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

New Algorithms: Based on LL^T and RR^T Factorizations

Consider the Cholesky foctorization 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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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} + 2 f_{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},
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&= \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},
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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

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

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The transformation formulas for the diagonal elements of A read

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

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

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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

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

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

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$$
\begin{aligned}
\hat{F}_2^T \hat{A} \hat{F}_2 &= \begin{bmatrix} f_{ii} & f_{ji} \\ 0 & 1 \end{bmatrix} \begin{bmatrix} a_{ii} & a_{ij} \\ a_{ij} & a_{jj} \end{bmatrix} \begin{bmatrix} f_{ii} & 0 \\ f_{ji} & 1 \end{bmatrix} \\
&= \begin{bmatrix} f_{ii}^2 a_{ii} + 2 f_{ii} f_{ji} a_{ij} + f_{ji}^2 a_{jj} & f_{ii} a_{ij} + f_{ji} a_{jj} \\ f_{ii} a_{ij} + f_{ji} a_{jj} & a_{jj} \end{bmatrix} \\
&= \begin{bmatrix} a_{ii} - \frac{2a_{ij} - (a_{ii} + a_{jj}) b_{ij}}{1 - b_{ij}^2} b_{ij} & \frac{a_{ij} - b_{ij} a_{jj}}{\sqrt{1 - b_{ij}^2}} \\ \frac{a_{ij} - b_{ij} a_{jj}}{\sqrt{1 - b_{ij}^2}} & a_{jj} \end{bmatrix},
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&= \frac{1}{\sqrt{1-b_{ij}^2}} \begin{bmatrix} c_\vartheta & -s_\vartheta \\ s_{\tilde{\vartheta}} & c_{\tilde{\vartheta}} \end{bmatrix}, \qquad \begin{aligned} c_{\tilde{\vartheta}} &= c_\vartheta \sqrt{1-b_{ij}^2} + s_\vartheta b_{ij}, \\ s_{\tilde{\vartheta}} &= s_\vartheta \sqrt{1-b_{ij}^2} - c_\vartheta b_{ij}. \end{aligned}
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It is easy to check that $c_{\tilde{\vartheta}}^2 + s_{\tilde{\vartheta}}^2 = 1$.

The algorithms based on LL^T and RR^T factorizations can be generalized to work with complex matrices

Definition of a Hybrid and a General Method

Definition

Let $\mathcal{H}$ denote a collection of Jacobi methods for the positive definite generalized eigenvalue problem $Ax = \lambda Bx$ which satisfy the following two rules:

1. at step k the pivot submatrix $\hat{A}^{(k)}$ is diagonalized and $\hat{B}^{(k)}$ is transformed to I_2,
2. at least one of the two diagonal elements of the pivot submatrix $\hat{F}_k$ is not smaller than $\sqrt{2}/2$.

An element of $\mathcal{H}$ is called a *general PGEP Jacobi method*. A *hybrid Jacobi method* is any method from $\mathcal{H}$ that uses at each step either the HZ, $LL^T J$ or $RR^T J$ algorithm.

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In this definition the pivot strategy is not specified, hence any can be used. If a Jacobi method uses only the HZ (LL^TJ, RR^TJ) algorithm, it will be called the HZ (LL^TJ, RR^TJ) method.

Some Remarks

- It is easy to show that HZ, LL^TJ and RR^TJ methods belong to the class $\mathcal{H}$.

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- Algorithms based on LL^T and RR^T factorizations have got their names $LL^T J$ and $RR^T J$ algorithm, because LL^T and RR^T factorizations are followed by one step of the Jacobi method for the symmetric matrix.
- The general (PGEP) Jacobi method can use at each step any conceivable algorithm which satisfies the above two rules. For example, it can use the FL method combined with normalization of the elements of B.

Some Remarks

- All real algorithms have the form

$$\hat{Z} = \frac{1}{\sqrt{1 - b_{ij}^2}} \begin{bmatrix} \cos\phi & -\sin\phi \\ \cos\psi & \sin\psi \end{bmatrix}.$$

  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 $b_{11} = \cdots = b_{nn}$ and the same condition for $\hat{Z}^T \hat{B} \hat{Z}$, then this form of $\hat{Z}$ is just the Gose's theorem.

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Later Hari generalized that result to complex matrices.

Global Convergence (Real and Complex Algorithm)

We have used the following measure in the convergence analysis:

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

The HZ method converges globally if

$$A^{(k)} \to \Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n), \quad B^{(k)} \to I_n \qquad \text{as} \quad k \to \infty,$$

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

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Then we have proved the global convergence 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:

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

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

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Theorem

If $S(B^{(0)}) < \dfrac{1}{n(n-1)}$ *and* $S(A^{(0)}, B^{(0)}) < \dfrac{\delta}{2\sqrt{1+\mu^2}}$,
then for the general cyclic and for the serial strategies it holds, respectively:

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

$$S(A^{(N)}, B^{(N)}) \;\leq\; \sqrt{1+\mu^2}\,\frac{S^2(A^{(0)}, B^{(0)})}{\delta}.$$

In the case of multiple eigenvalues, the method is not quadratically convergent, but can be modified to be such.

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Let

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

where $s_p = n$.

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where $s_p = n$. Then

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

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,

$$3\delta_r = \min_{\substack{1\leq t\leq p \\ t\neq r}} \mid \lambda_{s_r} - \lambda_{s_t} \mid, \quad 1 \leq r \leq p.$$

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Then $\quad \delta = \min_{1\leq r\leq p} \delta_r \quad$ 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, i.e. $A_{11}, \ldots, A_{pp}$ have orders $n_1, \ldots, n_p$, resp..
For a square matrix $X = (X_{rt})$ partitioned according to $n_1, \ldots, n_p$, let

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

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

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

Multiple Eigenvalues

Theorem (Hari 91)

Let $D_r + E_r = A - \lambda_{s_r} B$, $diag(E_r) = 0$, $1 \leq r \leq p$. *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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This impacts asymptotic convergence and accuracy of the algorithm.

Multiple Eigenvalues

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

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 $n \ge 3$, $p \ge 2$,

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

then

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

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- Hence we first present the algorithms, then theoretical background for the tests and then the results.
- One can hope for high relative accuracy of the methods only for well-behaved initial pairs (A, B).
- An example of such pairs are the pairs of positive definite symmetric matrices which can be well symmetrically scaled. These are the pairs for which the conditions $\kappa_2(\Delta_A A \Delta_A)$ and $\kappa_2(\Delta_B B \Delta_B)$ are small for some diagonal matrices Δ_A and Δ_B.

Algorithm HZ

select the pivot pair (i, j)
if $a_{ij} \neq 0$ or $b_{ij} \neq 0$ then

$$\rho = 0.5\,(\sqrt{1+b_{ij}} + \sqrt{1-b_{ij}}); \quad \xi = b_{ij}/(2\rho);$$
$$\tau = \sqrt{(1+b_{ij})(1-b_{ij})}; \quad t2 = 2a_{ij} - (a_{ii}+a_{jj})b_{ij};$$

if $t2 = 0$ then $t = 0$;
else

$$ct2 = \tau\,(a_{ii} - a_{jj})/t2;$$
$$t = \mathtt{sign}(ct2)/(\mathtt{abs}(ct2) + (1 + \sqrt{1+ct2^2});$$

end

$$cs = 1/\sqrt{1+t^2}; \qquad sn = t/\sqrt{1+t^2};$$
$$c1 = (\rho \cdot cs - \xi \cdot sn)/\tau; \qquad s1 = (\rho \cdot sn + \xi \cdot cs)/\tau;$$
$$c2 = (\rho \cdot cs + \xi \cdot sn)/\tau; \qquad s2 = (\rho \cdot sn - \xi \cdot cs)/\tau;$$
$$\delta_i = (b_{ij}/\tau - s1)(b_{ij}/\tau + s1)a_{ii} + (2c1\,a_{ij} + s2\,a_{jj})\,s2;$$
$$\delta_j = (s2 - b_{ij}/\tau)(s2 + b_{ij}/\tau)\,a_{jj} + (2c2\,a_{ij} - s1\,a_{ii})\,s1;$$
$$a'_{ij} = (c1\,c2 - s1\,s2)a_{ij} + (c2\,s2\,a_{jj} - c1\,s1\;a_{ii}); \quad a'_{ji} = a'_{ij};$$
$$b'_{ij} = 0; \quad b'_{ji} = b'_{ij}; \qquad a'_{ii} = a_{ii} + \delta_i; \quad a'_{jj} = a_{jj} - \delta_j;$$

for $k = 1, \ldots, n,\ k \neq i, j$ do

$$a'_{ki} = c1 \cdot a_{ki} + s2 \cdot a_{kj}; \quad b'_{ki} = c1 \cdot b_{ki} + s2 \cdot b_{kj}; \quad a'_{ik} = a'_{ki}; \quad b'_{ik} = b'_{ki};$$
$$a'_{kj} = c2 \cdot a_{kj} - s1 \cdot a_{ki}; \quad b'_{kj} = c2 \cdot b_{kj} - s1 \cdot b_{ki}; \quad a'_{jk} = a'_{kj}; \quad b'_{jk} = b'_{kj};$$

endfor

endif

Algorithm $LL^T J$

```
select the pivot pair (i, j)
if a_ij ≠ 0 or b_ij ≠ 0 then
```

$\beta = b_{ij}\,,\ \tau = \mathtt{sqrt}((1+\beta)(1-\beta));\quad \alpha = a_{ij} - \beta a_{ii}\,;$

$\quad$ `if` $\ \alpha = 0\ $ `then` $\ t = 0;$

$\quad$ `else` $\ ct2 = (0.5\,(a_{ii} - a_{jj}) + \alpha\beta)/(\alpha\,\tau);$

$\qquad t = \mathtt{sign}(ct2)/(\mathtt{abs}(ct2) + \mathtt{sqrt}(1 + ct2^2));$

$\quad$ `endif`

$\quad cs = 1/\mathtt{sqrt}(1+t^2);\quad sn = t/\mathtt{sqrt}(1+t^2);$

$\quad c1 = cs - sn\,\beta/\tau\,;\quad s1 = sn + cs\,\beta/\tau\,;\quad c2 = cs/\tau\,;\quad s2 = sn/\tau\,;$

$\quad \delta_i = t\alpha/\tau\,;\quad \delta_j = (\,t\alpha + (\beta/\tau)\cdot(2a_{ij} - (a_{ii}+a_{jj})\beta)\,)/\tau\,;$

$\quad a'_{ij} = (c1\,c2 - s1\,s2)\,a_{ij} + (c2\,s2\,a_{jj} - c1\,s1\,a_{ii});\quad a'_{ji} = a'_{ij}\,;$

$\quad b'_{ij} = (c1\,c2 - s1\,s2)\,\beta + (c2\,s2 - c1\,s1);\quad b'_{ji} = b'_{ij}\,;$

$\quad a'_{ii} = a_{ii} + \delta_i\,;\quad a'_j = a_{jj} - \delta_j\,;$

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$\quad$ `endfor`

`endif`

Algorithm RR^TJ

```
select the pivot pair (i, j)
if a_ij ≠ 0 or b_ij ≠ 0 then
    β = b_ij,  τ = sqrt((1 + β)(1 − β));   α = a_ij − β a_jj;
    if  α = 0   then  t = 0;
    else  ct2 = (0.5 (a_ii − a_jj) − αβ)/(α τ);
              t = sign(ct2)/(abs(ct2) + sqrt(1 + ct2^2));
    endif
    cs = 1/sqrt(1 + t^2);   sn = t/sqrt(1 + t^2);
    c1 = cs/τ;   s1 = sn/τ;   c2 = cs + sn β/τ;   s2 = sn − cs β/τ;
    δ_j = tα/τ;   δ_i = ( tα − (β/τ) · (2a_ij − (a_ii + a_jj)β) )/τ;
    a'_ij = (c1 c2 − s1 s2) a_ij + (c2 s2 a_jj − c1 s1 a_ii);   a'_ji = a'_ij;
    b'_ij = (c1 c2 − s1 s2) β + (c2 s2 − c1 s1);   b'_ji = b'_ij;
    a'_ii = a_ii + δ_i;   a'_j = a_jj − δ_j;
    for k = 1, ..., n, k ≠ i, j  do
      a'_ki = c1 · a_ki + s2 · a_kj;   b'_ki = c1 · b_ki + s2 · b_kj;   a'_ik = a'_ki;   b'_ik = b'_ki
      a'_kj = c2 · a_kj − s1 · a_ki;   b'_kj = c2 · b_kj − s1 · b_ki;   a'_jk = a'_kj;   b'_jk = b'_kj;
    endfor
endif
```

Theorem (Theorem 3.2, Drmač 1998)

Let $A = A^T \succ O$, $B = B^T \succ O$ *and* $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ *be the eigenvalues of the pair* (A, B).
Let $A_S = D_A^{-1/2} A D_A^{-1/2}$, $B_S = D_B^{-1/2} B D_B^{-1/2}$, $D_A = diag(A)$, $D_B = diag(B)$.
Let δA *and* δB *be symmetric perturbations such that*

$$\|(\delta A)_S\|_2 \|A_S^{-1}\|_2 < 1 \quad \text{and} \quad \|(\delta B)_S\|_2 \|B_S^{-1}\|_2 < 1,$$

where $(\delta A)_S = D_A^{-1/2} \delta A D_A^{-1/2}$, $(\delta B)_S = D_B^{-1/2} \delta B D_B^{-1/2}$.
If $\tilde{\lambda}_1 \geq \tilde{\lambda}_2 \geq \cdots \geq \tilde{\lambda}_n$ *are th eigenvalues of* $(A + \delta A, B + \delta B)$, *then*

$$\max_{1 \leq i \leq n} \frac{|\tilde{\lambda}_i - \lambda_i|}{\lambda_i} \leq \frac{\|(\delta A)_S\|_2 \|A_S^{-1}\|_2 + \|(\delta B)_S\|_2 \|B_S^{-1}\|_2}{1 - \|(\delta B)_S\|_2 \|B_S^{-1}\|_2} = \frac{\varepsilon_{A_S} \kappa_2(A_S) + \varepsilon_{B_S} \kappa_2(B_S)}{1 - \varepsilon_{B_S} \kappa_2(B_S)},$$

where $\varepsilon_{A_S} = \|(\delta A)_S\|_2 / \|A_S\|_2$, $\varepsilon_{B_S} = \|(\delta B)_S\|_2 / \|B_S\|_2$, *and* $\kappa_2(X)$ *is the spectral condition number of* X.

Theoretical Background

- For all considered methods the starting matrix $B^{(0)}$ is just B_S. Therefore

$$\max_{1\leq i\leq n} \frac{|\tilde{\lambda}_i - \lambda_i|}{\lambda_i} \leq \frac{\varepsilon_{A_S}\kappa_2(A_S) + \varepsilon_{B^{(0)}}\kappa_2(B_S)}{1 - \varepsilon_{B_S}\kappa_2(B^{(0)})},$$

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- For these well-behaved pairs we have to find out the methods which generate at every step only tiny relative errors $\varepsilon_{A_S^{(k)}}$, $\varepsilon_{B_S^{(k)}}$ and in the same time matrices with small or modest condition numbers $\kappa_2(A_S^{(k)})$ and $\kappa_2(B^{(k)})$.

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- For all considered methods the starting matrix $B^{(0)}$ is just B_S. Therefore

$$\max_{1\le i\le n} \frac{|\tilde{\lambda}_i - \lambda_i|}{\lambda_i} \le \frac{\varepsilon_{A_S}\kappa_2(A_S) + \varepsilon_{B^{(0)}}\kappa_2(B_S)}{1 - \varepsilon_{B_S}\kappa_2(B^{(0)})},$$

- The initial normalization $B \mapsto B_S = B^{(0)}$, simplifies the algorithm. Moreover, it has a stabilizing effect on the iterative process, because it almost optimally reduces the condition of B and all $B^{(k)}$, $k \ge 1$ will have almost best possible conditions. Van der Sluis, A.: Condition numbers and equilibration of matrices. Numer. Math. 14 (1), 14–23 (1969)
- For these well-behaved pairs we have to find out the methods which generate at every step only tiny relative errors $\varepsilon_{A_S^{(k)}}$, $\varepsilon_{B_S^{(k)}}$ and in the same time matrices with small or modest condition numbers $\kappa_2(A_S^{(k)})$ and $\kappa_2(B^{(k)})$.

Nonetheless, this is a demanding task, so we shall go for a shortcut.

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- The relation (5) should hold irrespectively of how large is the condition $\kappa_2(A^{(0)})$. Therefore, we are interested in how $\varrho_{(A,B)}$ behaves with respect to $\chi_{(A,B)}$,

$$\chi_{(A,B)} := \kappa_2(A^{(0)}, B^{(0)}) = \sqrt{\kappa_2^2(A^{(0)}) + \kappa_2^2(B^{(0)})}.$$

- For the given sample of well behaved pairs Υ, and for each method, we shall make its graph of relative errors: $\mathcal{E}$,

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- The method will be considered to be high relative accurate if the ordinates of the points on the graph are of order $\mathcal{O}(\mathbf{u})$ where $\mathbf{u} \approx 2.2 \cdot 10^{-16}$.

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where D_A and D_B are the diagonal parts of A and B. Then $\kappa_2(A_S^{(0)})$ and $\kappa_2(B^{(0)})$ can be controlled by the diagonal elements of Δ_A, Δ_B, Σ, since

$$\kappa_2(A_S^{(0)}) \leq n\kappa_2^2(\Sigma)\kappa_2(\Delta_A) \quad \text{and} \quad \kappa_2(B^{(0)}) \leq n\kappa_2^2(\Sigma)\kappa_2(\Delta_B),$$

although most often $\kappa_2(A_S^{(0)})$ and $\kappa_2(B^{(0)})$ are much smaller than these bounds.

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If we set $\Delta = I_n$ i $(A^{(0)}, B^{(0)}) = (D_B^{-1/2} A D_B^{-1/2}, B_S)$, then we know in advance the eigenvalues of $(A^{(0)}, B^{(0)})$ These are the quotients

$$(\Delta_A)_{jj}/(\Delta_B)_{jj}, \qquad 1 \leq j \leq n.$$

This way can be used when considering behavior of the methods on pairs with multiple eigenvalues.

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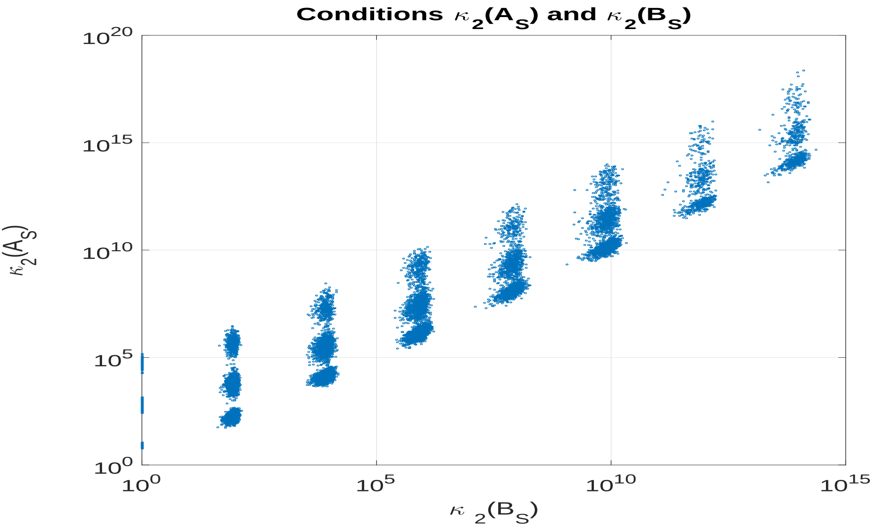
- We have generated the sample Υ of 18900 pairs of matrices of order 10. As "exact eigenvalues" we have used the eigenvalues computed by the M-function `eig(A,B)` in variable precision arithmetic (VPA) using 80 decimal digits.

Matrix conditions



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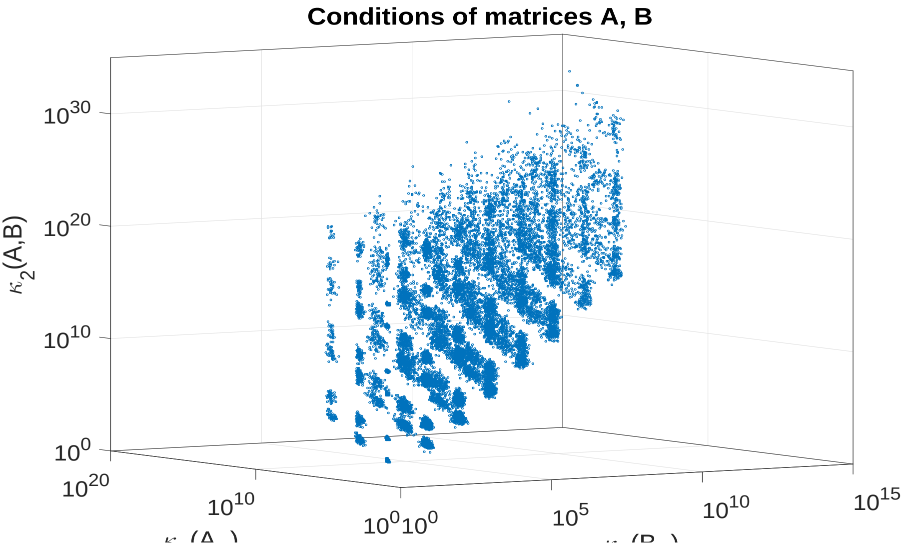
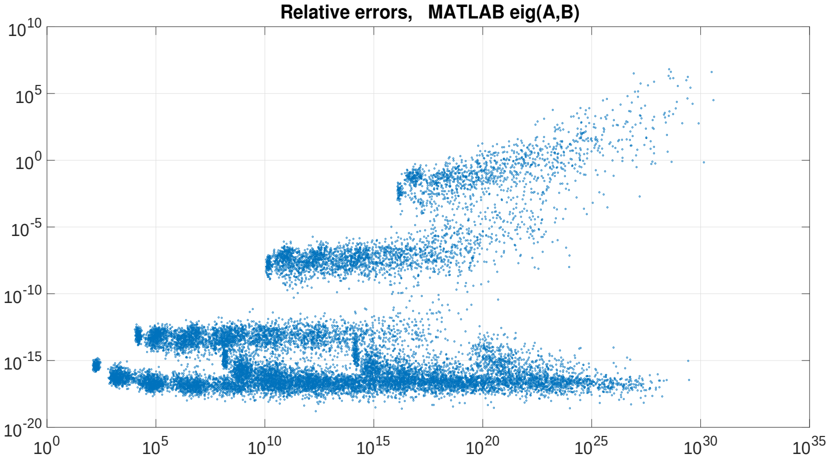
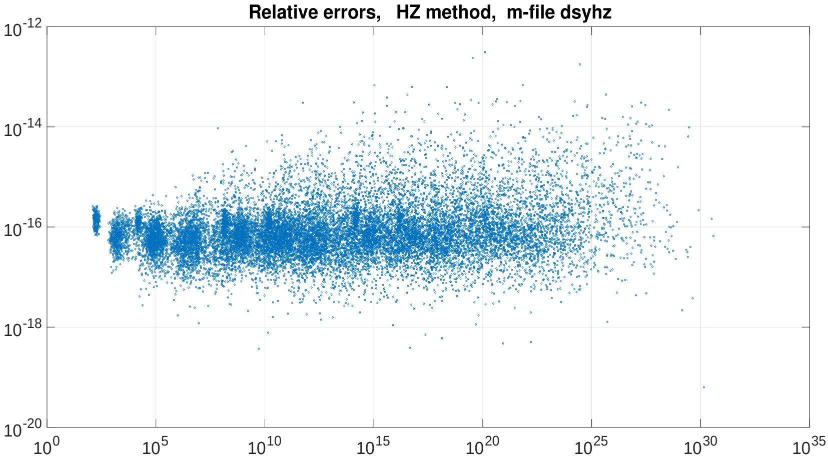


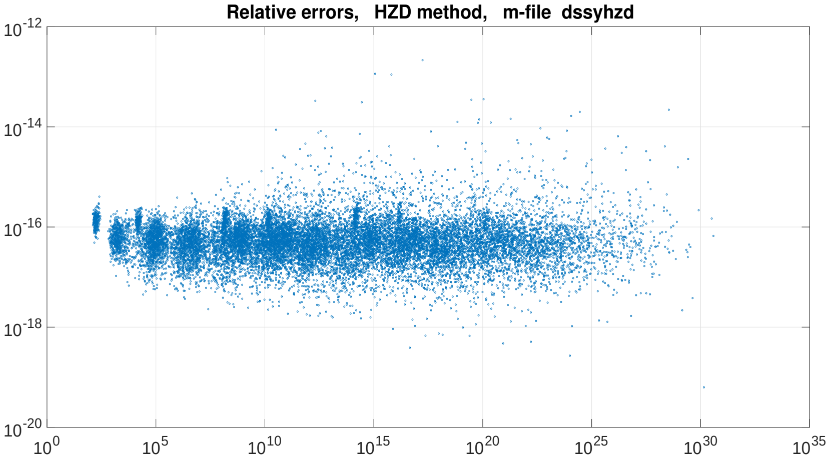
Relative errors: MATLAB eig function



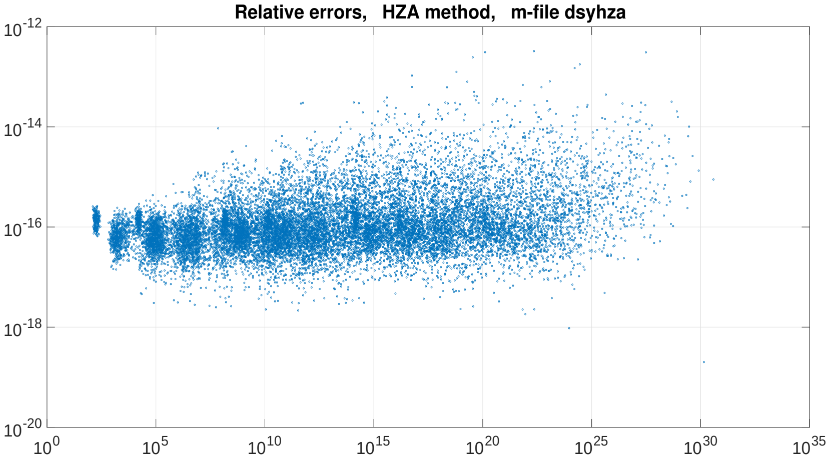
Relative errors: HZ method



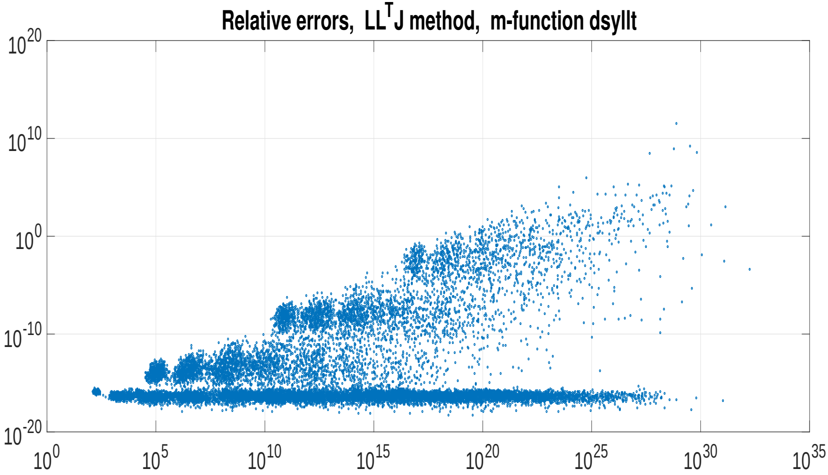
Relative errors: HZD method



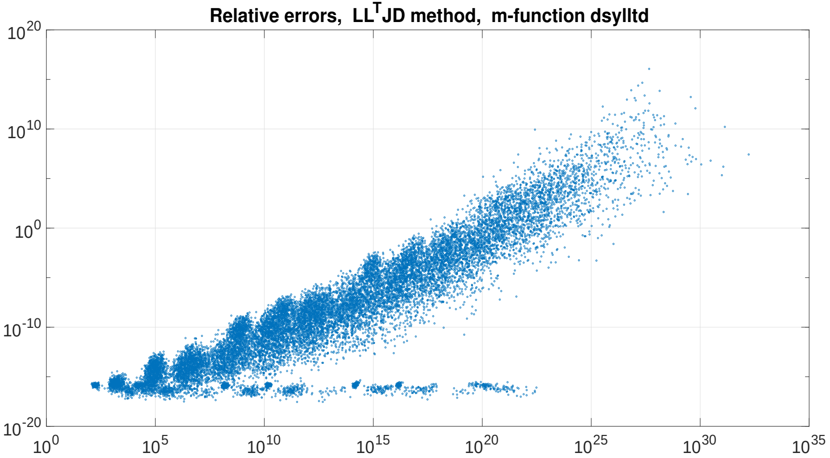
Relative errors: HZA method



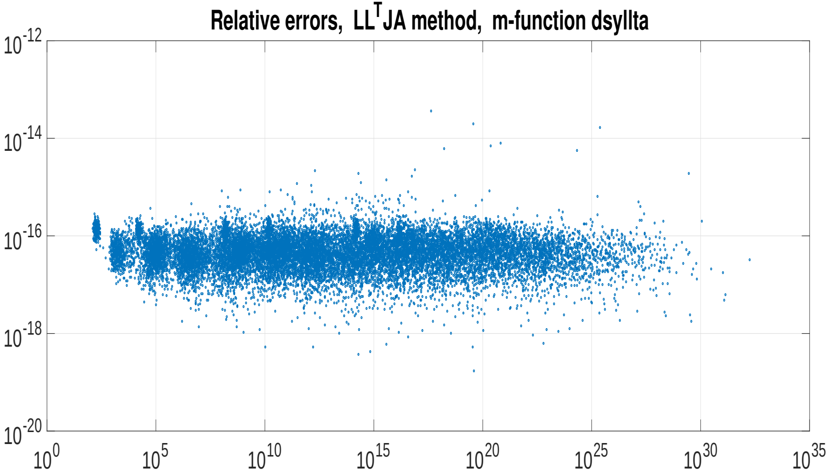
Relative errors: $LL^T J$ method



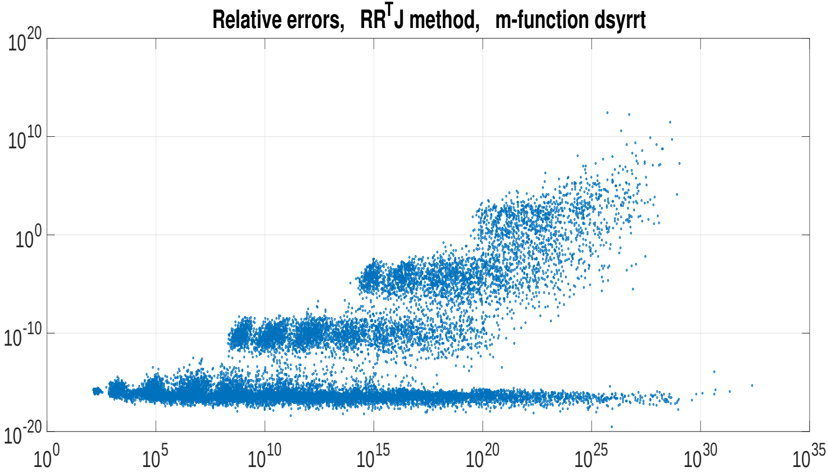
Relative errors: Descending LL^TJ method



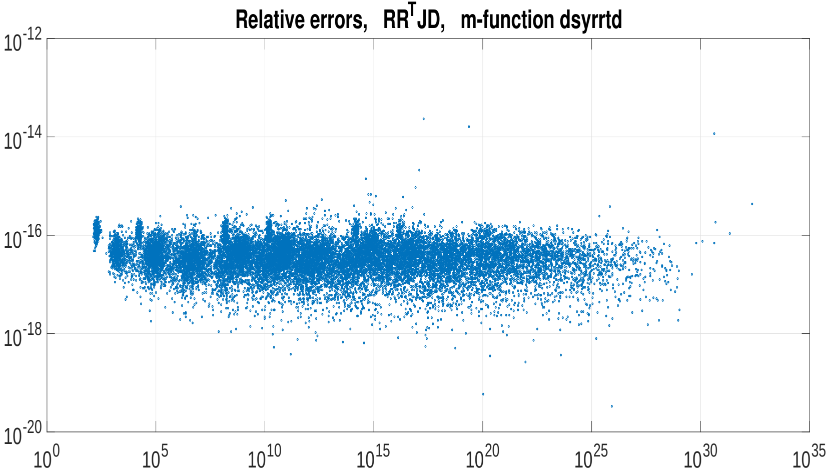
Relative errors: Ascending $LL^T J$ method



Relative errors: $RR^T J$ method



Relative errors: Descending RR^TJ method



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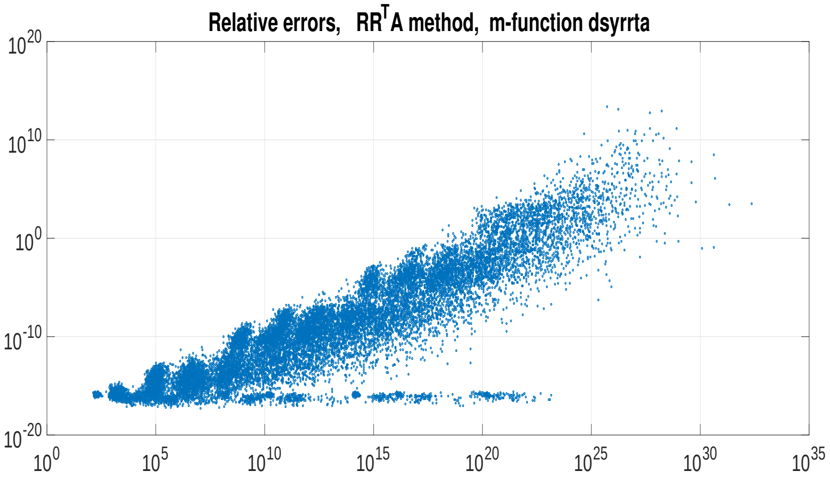

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We complete our presentation with the graph associated with the CJ method.

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