On Element-wise and Block-wise Jacobi Methods for PGEP

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- Since we consider theoretical aspects of the methods, we have restricted our attention to element-wise, two-sided Jacobi-type methods for PGEP. They can be used standalone or as kernel algorithms for the block methods.

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For such a pair (A, B) there exists a nonsingular matrix F such that

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where $I_n = [e_1, \ldots, e_n]$.

How to Solve PGEP?

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

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

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If L has small singular value(s), then the computed $L^{-1}AL^{-*}$ will have corrupt eigenvalues. Then one can try to maximize the minimum eigenvalue of B by rotating the pair

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

(ask Bart Vandereycken about it) and then derive a method which works with the initial pair (A, B).

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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.

The FL Method (what is known, what is not known?)

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- What is missing?
  1. Some global convergence proof
  2. Some proof of high relative accuracy of the method on well-behaved matrix pairs
  3. Complex algorithm for definite pairs of Hermitian matrices

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  3. Connection of the complex HZ method to the complex FL method

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- V. Hari and E. Begović Kovač have developed tools (block-Jacobi annihilators and operators) for proving the global convergence of real and complex block and element-wise Jacobi methods for PGEP and similar problems under the class of generalized serial strategies (ETNA 46, 2017, and one work in progress)

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  However, we are confident that a robust algorithm with overall good properties can be found
- To find the best possible candidate for the kernel algorithm for one-sided block Jacobi methods for GSVD, in the real and in the complex case
- To make sound global and asymptotic convergence proofs of the block Jacobi methods for PGEP

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The problem with block methods is that they need best possible kernel algorithms: globally convergent, highly accurate and numerically fast.

Returning to Element-wise PGEP Jacobi Methods

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For obvious reasons we shall try to escape derivation of complex algorithms!!!

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$$Z_k = \begin{bmatrix} I & & & & \\ & c_k & & -s_k & \\ & & I & & \\ & \tilde{s}_k & & \tilde{c}_k & \\ & & & & I \end{bmatrix} \begin{matrix} \\ i(k) \\ \\ j(k) \\ \\ \end{matrix}, \qquad c_k^2 + s_k^2 = \tilde{c}_k^2 + \tilde{s}_k^2 = 1/\sqrt{1 - b_{i(k)j(k)}^2}.$$

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

Derivation of the HZ Method

At step k we denote: $A^{(k)} \mapsto A, \quad A^{(k+1)} \mapsto A', \quad Z_k \mapsto Z,$

$$\hat{A} = \begin{bmatrix} a_{ii} & a_{ij} \\ a_{ij} & a_{jj} \end{bmatrix}, \quad \hat{B} = \begin{bmatrix} 1 & b_{ij} \\ b_{ij} & 1 \end{bmatrix}, \quad \hat{Z} = \begin{bmatrix} c & -s \\ \tilde{s} & \tilde{c} \end{bmatrix}.$$

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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 approaches yield the same algorithm.

Essential Part of the Algorithm

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

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

Essential Part of the Algorithm

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

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

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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!

$$2\rho\xi = b_{ij}, \quad |\xi| \le \sqrt{2}/2 \le \rho \le 1$$

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

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

There are more formulas!

Let

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

then

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

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

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

There are more formulas!

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

We also have

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

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

Algorithm HZ

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

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

$$c1 = (\rho\cdot cs - \xi\cdot sn)/\tau;\quad s1 = (\rho\cdot sn + \xi\cdot cs)/\tau;$$

$$c2 = (\rho\cdot cs + \xi\cdot sn)/\tau;\quad s2 = (\rho\cdot sn - \xi\cdot cs)/\tau;$$

$$\delta_i = (b_{ij}/\tau - s1)(b_{ij}/\tau + s1)a_{ii} + (2c1\,a_{ij} + s2\,a_{jj})\,s2;$$

$$\delta_j = (s2 - b_{ij}/\tau)(s2 + b_{ij}/\tau)\,a_{jj} + (2c2\,a_{ij} - s1\,a_{ii})\,s1;$$

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

$$b'_{ij} = 0;\quad b'_{ji} = b'_{ij};\quad a'_{ii} = a_{ii} + \delta_i;\quad a'_{jj} = a_{jj} - \delta_j;$$

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

Digression: Complex Matrices

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

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$$A' = Z^* A Z, \quad B' = Z^* B Z.$$

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

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

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

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

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

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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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Assuming $c > 0$, one obtains $\quad a = b_{ij}, \;\; c = \sqrt{1 - b_{ij}^2}, \quad$ hence

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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

$$\hat{F}_1 = \hat{L}^{-T}, \quad then \quad \hat{F}_1^T \hat{B} \hat{F}_1 = I_2$$

and

The Algorithm Based on LL^T Factorization

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

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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

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

The Algorithm Based on LL^T Factorization

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The transformation formulas for the diagonal elements of A read

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

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

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

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If $a_{ii} = a_{jj}$, $a_{ij} = a_{ii}b_{ij}$ then ϑ is determined from $0/0$, 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

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

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

Algorithm LL^TJ

select the pivot pair (i, j)

if $a_{ij} \neq 0$ or $b_{ij} \neq 0$ then

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

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

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

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

endif

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

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

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

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

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

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

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

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

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

The Algorithm Based on RR^T Factorizations

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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

The Algorithm Based on RR^T Factorization

$$\hat{F}_2^T \hat{A} \hat{F}_2 = \begin{bmatrix} a_{ii} - \frac{2a_{ij} - (a_{ii} + a_{jj}) b_{ij}}{1 - b_{ij}^2} b_{ij} & \frac{a_{ij} - b_{ij} a_{jj}}{\sqrt{1 - b_{ij}^2}} \\ \frac{a_{ij} - b_{ij} a_{jj}}{\sqrt{1 - b_{ij}^2}} & a_{jj} \end{bmatrix}.$$

The final $\hat{F}$ has the form $\hat{F} = \hat{F}_2 \hat{J}$, where $\hat{J}$ is the Jacobi transformation which diagonalizes $\hat{F}_2^T \hat{A} \hat{F}_2$. Its angle ϑ is determined by the formula:

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

The Algorithm Based on RR^T Factorization

The transformation formulas for the diagonal elements of A read

$$
\begin{aligned}
a'_{ii} &= a_{ii} - \frac{2a_{ij} - (a_{ii} + a_{jj})b_{ij}}{1 - b_{ij}^2} b_{ij} + \tan\vartheta \cdot \frac{a_{ij} - a_{jj} b_{ij}}{\sqrt{1 - b_{ij}^2}}, \\
a'_{jj} &= a_{jj} - \tan\vartheta \cdot \frac{a_{ij} - a_{jj} b_{ij}}{\sqrt{1 - b_{ij}^2}}.
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a'_{jj} &= a_{jj} - \tan\vartheta \cdot \frac{a_{ij} - a_{jj}b_{ij}}{\sqrt{1 - b_{ij}^2}}.
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$$

If $a_{ii} = a_{jj}$, $a_{ij} = a_{jj}b_{ij}$ then we choose $\vartheta = 0$ and then a'_{ii} and a'_{jj} reduce to a_{ii} and a_{jj}, respectively.

The Algorithm Based on RR^T Factorization

This leads to the transformation matrix

$$\hat{Z} = \frac{1}{\sqrt{1-b_{ij}^2}} \begin{bmatrix} 1 & 0 \\ -b_{ij} & \sqrt{1-b_{ij}^2} \end{bmatrix} \begin{bmatrix} c_\vartheta & -s_\vartheta \\ s_\vartheta & c_\vartheta \end{bmatrix}$$

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

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

Algorithm RR^TJ

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

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

$\mathtt{if}\ \ \alpha = 0 \quad \mathtt{then}\ \ t = 0;$

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

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

$\mathtt{endif}$

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

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

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

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

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

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

$\mathtt{for}\ \ k = 1, \ldots, n,\ k \neq i, j \quad \mathtt{do}$

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

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

$\mathtt{endfor}$

$\mathtt{endif}$

Definition of a Hybrid and a General Method

Definition

Let $\mathcal{H}$ denote collection of Jacobi methods for PGEP $Ax = \lambda Bx$ which satisfy the following two rules:

1. at step k, $\hat{A}^{(k)}$ is diagonalized and $\hat{B}^{(k)}$ is transformed to I_2,
2. at least one diagonal element of $\hat{F}_k$ 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 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, $LL^T J$ and $RR^T J$ methods belong to $\mathcal{H}$

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- Algorithms based on LL^T and RR^T factorizations are called $LL^T J$ and $RR^T J$ algorithm, because LL^T and RR^T factorizations are followed by one step of the standard Jacobi method
- 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

$$\hat{Z} = \frac{1}{\sqrt{1 - b_{ij}^2}} \left[\begin{array}{cc} \cos\phi & -\sin\phi \\ \cos\psi & \sin\psi \end{array} \right].$$

  This follows from a result of Gose (ZAMM 59, 1979), who found the general form of a matrix $\hat{Z}$ which diagonalizes a $\hat{B} \succ O$ 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 for $\hat{Z}^T \hat{B} \hat{Z}$, then this form of $\hat{Z}$ is just the Gose's theorem.

Global Convergence of the General PGEP Jacobi Method

We have used the following measure in the convergence analysis:

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

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The general PGEP method is globally convergent if

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

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Actually, it is sufficient to show that $S(A, B) \to 0$ as $k \to \infty$.

We have proved the global convergence for the class of

- serial pivot strategies
- generalized serial strategies which includes all weakly wavefront strategies and many others (Hari, Begović Kovač, ETNA 46 (2017) 107-147)

Asymptotic Convergence for the HZ Method

Let (A, B) have simple eigenvalues:

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

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

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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.

Stability and High Relative Accuracy

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  First theoretical background for the tests, and then the test results
- High relative accuracy of the methods can be obtained only for well-behaved initial pairs (A, B)
- An example of such pairs are the pairs for which the condition numbers $\kappa_2(\Delta_A A \Delta_A)$ and $\kappa_2(\Delta_B B \Delta_B)$ are small for some diagonal matrices Δ_A and Δ_B.

Theorem

Let $A = A^T \succ O$, $B = B^T \succ O$ *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 symmetric 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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$$\varepsilon_{A_S} = \|(\delta A)_S\|_2 / \|A_S\|_2, \quad \varepsilon_{B_S} = \|(\delta B)_S\|_2 / \|B_S\|_2$$

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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

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

Theoretical Background

- 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 $B^{(k)}$, $k \geq 1$.
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- For those well-behaved pairs we have to find out what methods 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 $\kappa_2(A_S^{(k)})$ and $\kappa_2(B^{(k)})$.

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

How to detect high relative accuracy of a method?

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

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

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We can check numerically whether the inequality

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$$\varrho_{(A,B)} \le f(n)\mathbf{u}, \tag{3}$$

holds for a larger sample Υ of pairs (A,B). Here

- $\tilde{\lambda}_i$, $1 \le i \le n$ are computed eigenvalues of $(A^{(0)}, B^{(0)})$
- $f(n)$ is a slowly growing function of n and $\mathbf{u}$ is the unit round off
- The relation (3) should hold irrespectively of how large $\kappa_2(A^{(0)})$ is.

Therefore, we are interested in how $\varrho_{(A,B)}$ behaves with respect to $\chi_{(A,B)}$,

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

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- For the given sample of pairs Υ, and for each method, we shall make its graph of relative errors:

$$\mathcal{E} = \{(\chi_{(A,B)}\ ,\ \varrho_{(A,B)}) \,:\, (A, B) \in \Upsilon\}.$$

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

How to generate matrix pairs?

The starting pair $(A^{(0)}, B^{(0)})$ is generated by

- 4 the diagonal matrices : Δ_A, Δ_B, Σ, Δ and
- 2 orthogonal matrices U, V of order n.

It is done in two steps:

1: $F = U\Sigma V^T, \quad A = F^T \Delta_A F, \quad B = F^T \Delta_B F,$

2: $B^{(0)} = B_S = D_B^{-1/2} B D_B^{-1/2}, \quad A^{(0)} = \Delta A_S \Delta,\ A_S = D_A^{-1/2} A D_A^{-1/2},$

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.

How to generate matrix pairs?

To simplify the construction we set $\Delta_B = I_n$.

If the method is high relative accurate, then $\varrho_{(A,B)}$ from the relation (3) should not depend on $\kappa_2(\Delta)$.

Note that

$$\kappa_2(A^{(0)}) \leq \kappa_2(A_S^{(0)})\kappa_2^2(\Delta).$$

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.

More Details

- Diagonal matrices are constructed by help of the M-function `diag(d)`
- `d` is a vector, and vectors are constructed by the M-function `logspace(x1,x2,n)`. We use it for the diagonal matrices Σ and Δ_A.
- For the construction of Δ we use our m-function

  `scalvec(k1,k2,k3,n,k)`

  which generates vector of length n, $d = [10^{\mathtt{k1}}, \ldots, 10^{\mathtt{k2}}, \ldots, 10^{\mathtt{k3}}]$ where `k` determines the position of $10^{\mathtt{k2}}$ within the components of d.
- To compute Δ, the function `scalvec` is used within triple loop controlled by the indices `k1`, `k2` and `k3`
- Orthogonal matrices U and V are computed by the command

  `[Q,~]=qr(rand(n))`
- 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.

The Methods and Their Variants

For each of the methods, HZ, LL^TJ, RR^TJ, we have made two additional variants. Let us explain it for the case of the HZ method.

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We have used deRijk serial strategy. This is modified row-cyclic strategy:

$$\begin{bmatrix} \bullet & 1 & 2 & 3 & 4 & 5 \\ & \bullet & 6 & 7 & 8 & 9 \\ & & \bullet & 10 & 11 & 12 \\ & & & \bullet & 13 & 14 \\ & & & & \bullet & 15 \\ & & & & & \bullet \end{bmatrix}$$

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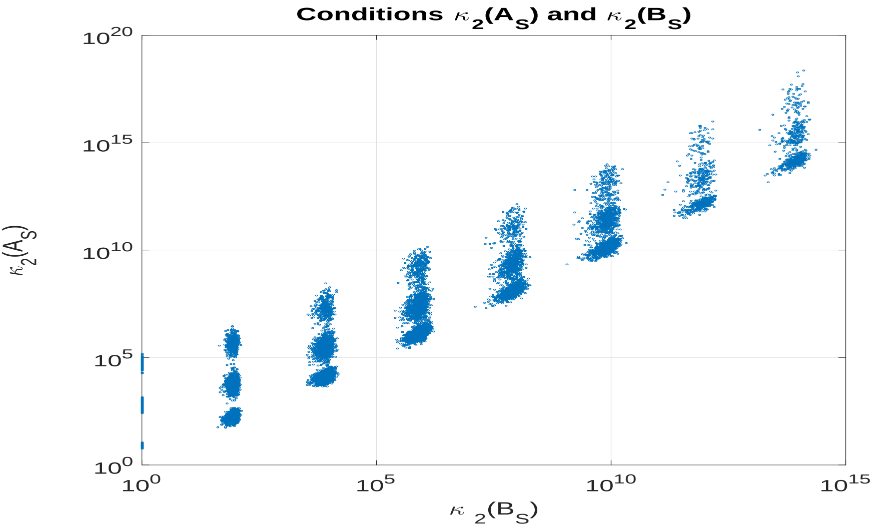
We call it descending HZ method or shorter HZD method, because the diagonal elements tend to end in descending order. In the similar way is defined ascending HZ method or HZA method.

Matrix conditions



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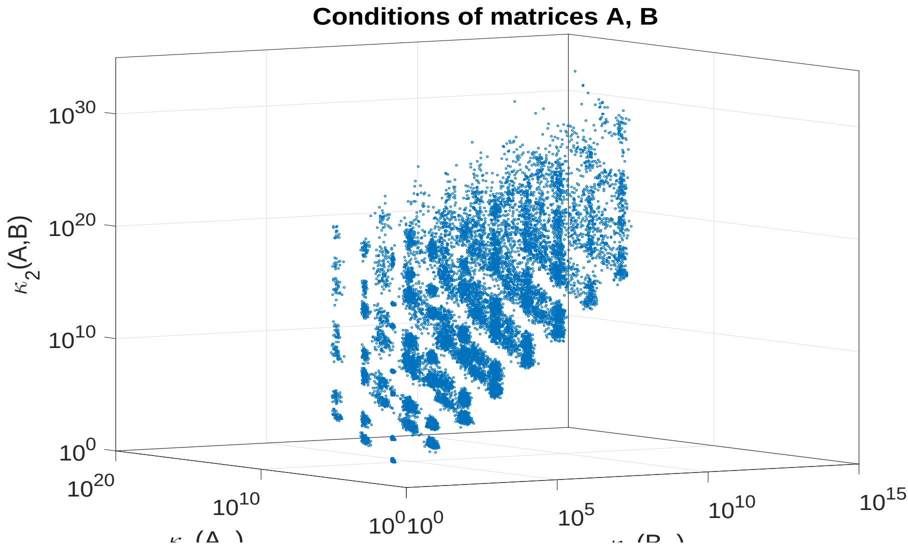
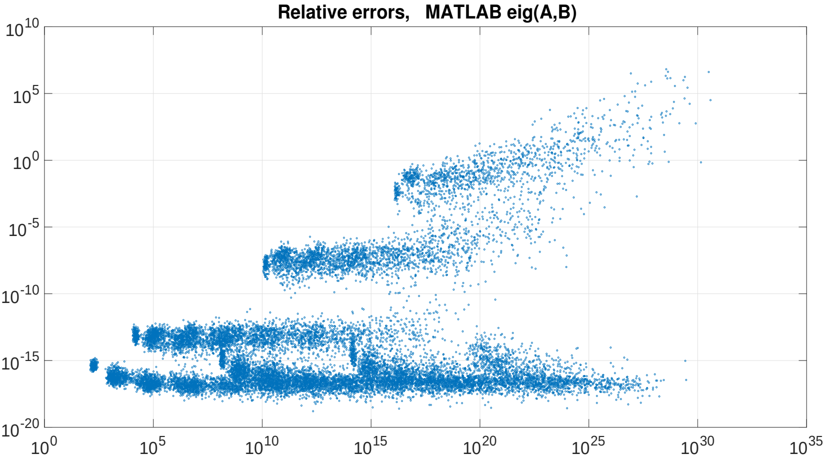
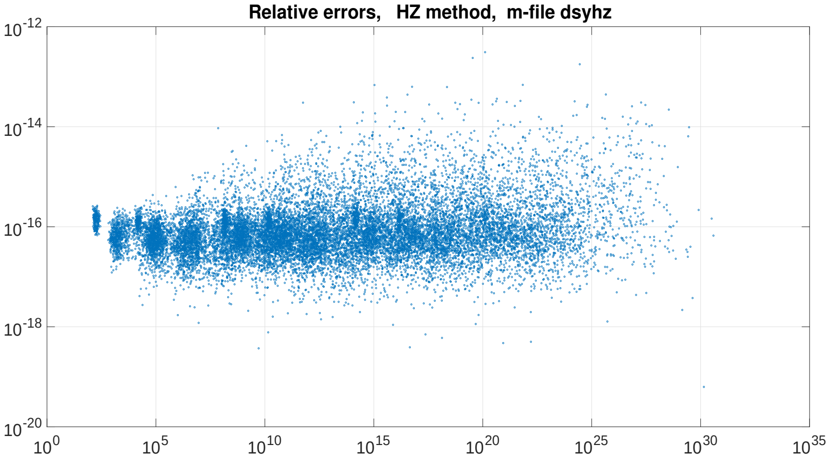


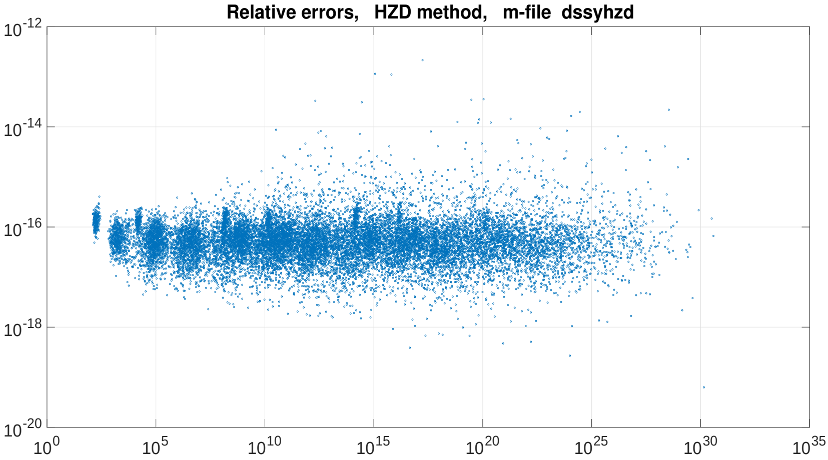
Relative errors: MATLAB eig function



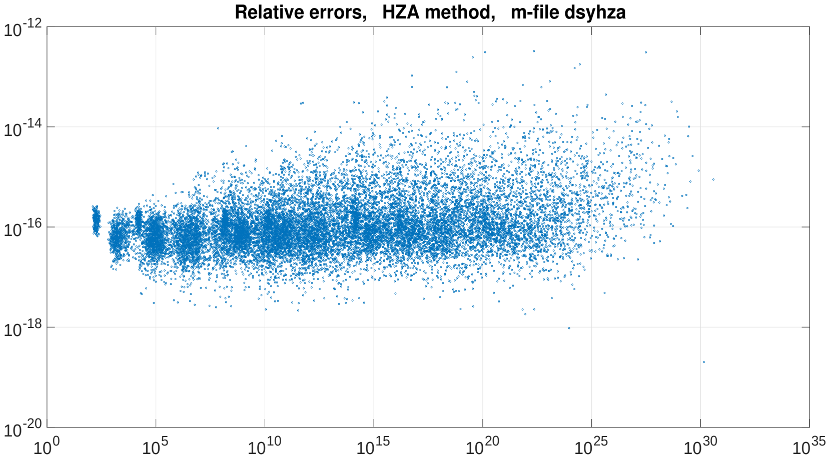
Relative errors: HZ method



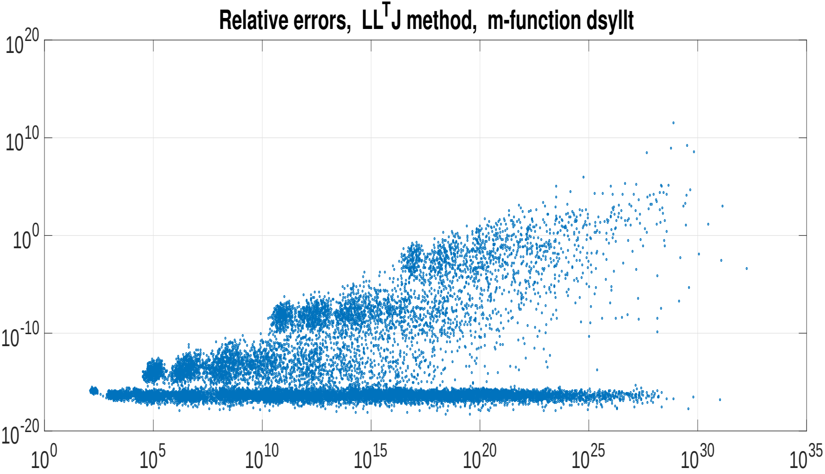
Relative errors: HZD method



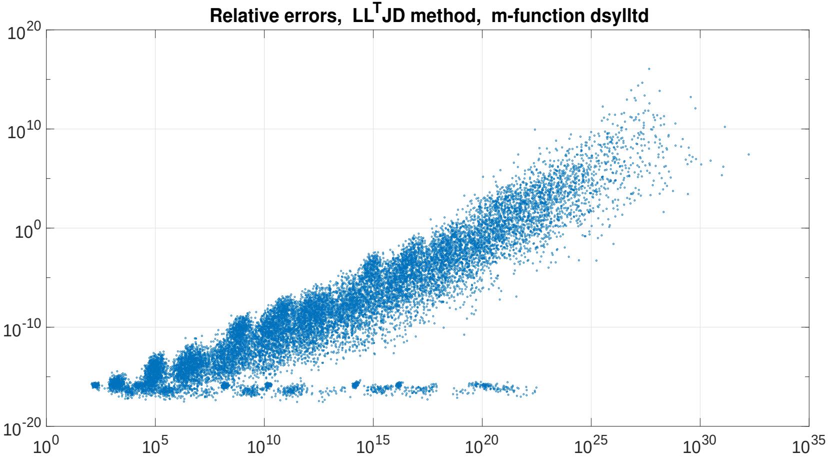
Relative errors: HZA method



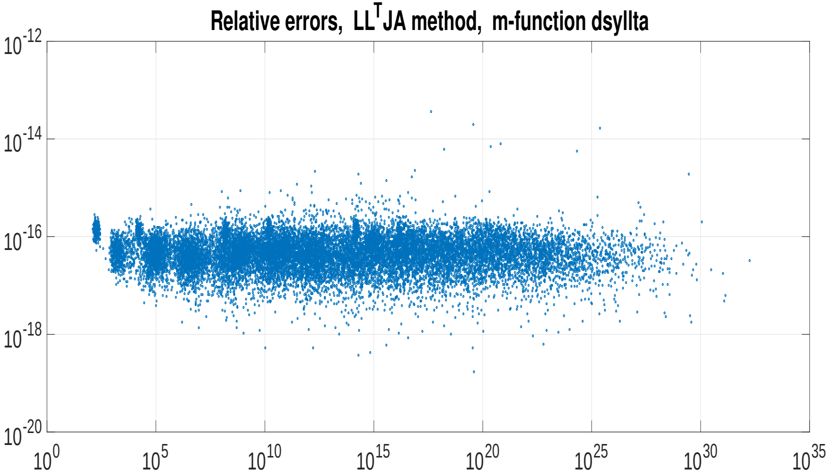
Relative errors: $LL^T J$ method



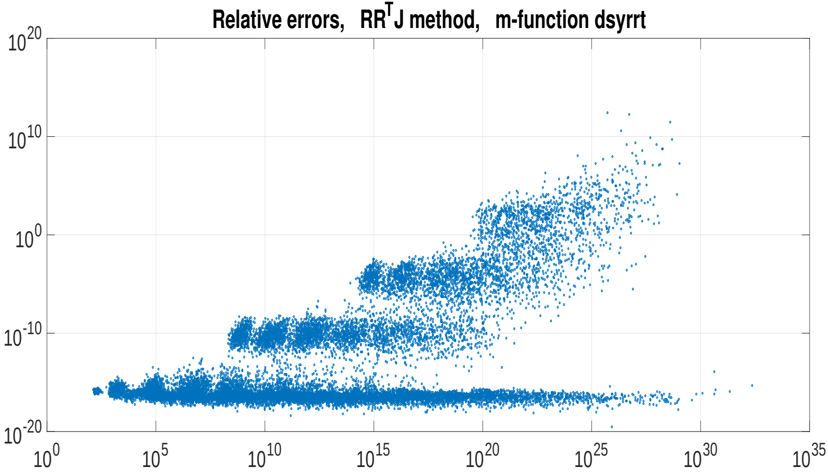
Relative errors: Descending LL^TJ method



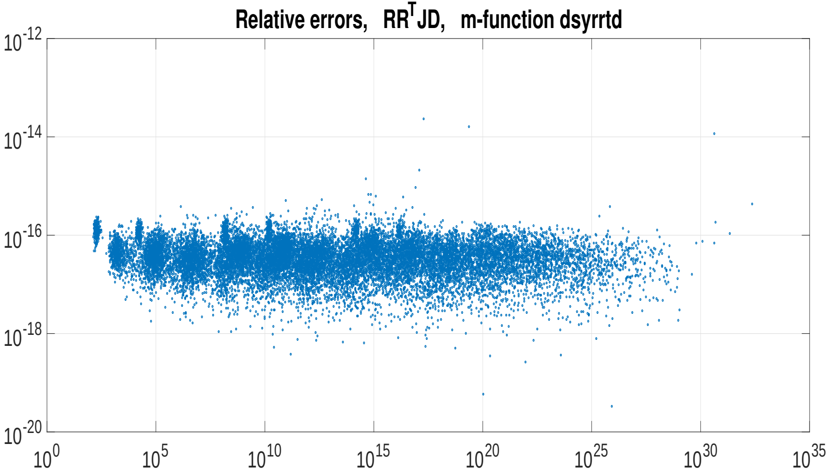
Relative errors: Ascending LL^TJ method



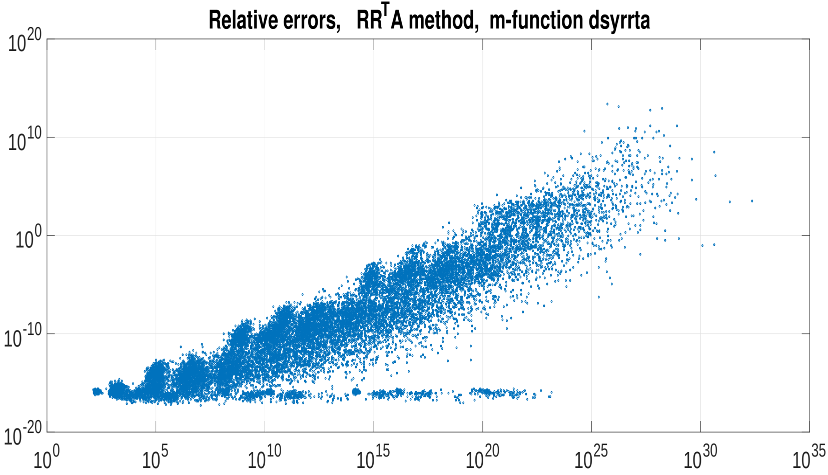
Relative errors: RR^TJ method



Relative errors: Descending RR^TJ method



Relative errors: Ascending RR^TJ method



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We see that just one variant of LL^TJ method (LL^TJA) and just one variant of RR^TJ method (RR^TJD) is indicated as relatively accurate.

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%%% Algorithm CJ

choose the pivot pair (i, j)

if $a_{ii} \geq a_{jj}$ **then** select $LL^T J$ algorithm
else select $RR^T J$ algorithm

endif

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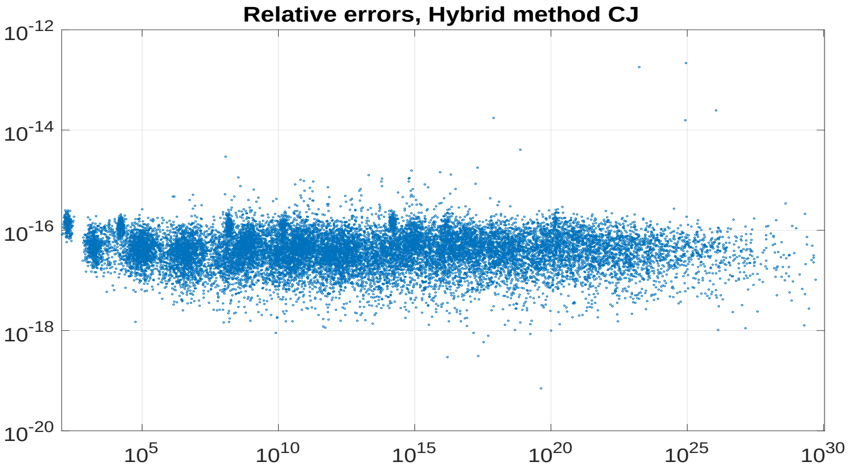
We end this presentation with the graph associated with the CJ method.

Relative errors: *CJ* method



Thank you for your time