## Diagonalization Methods for Solving Definite Generalized Eigenvalue Problem

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• GEP (DGEP, PGEP)

This work has been fully supported by Croatian Science Foundation under the project



IP-09-2014-3670.



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- Global convergence of block algorithms

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- The theoretical aspects of one-sided methods can be better analysed and understood if they are considered/imagined as two-sided methods
- One-sided methods have problem with terminating the process. Stopping of the process can be costly, especially if the matrix dimension *n* is large.
- Two sided methods can smoothly, timely and cost effectively stop the process.

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

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## Why are Element-wise Methods Important?

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Hence, probably the best choice for the kernel algorithm is some element-wise diagonalization method.

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

## The Real and Complex FL Method

Starting with a definite pair (A, B) of Hermitian matrices, FL generates a sequence of "congruent" matrix pairs

$$(A,B) = (A^{(0)}, B^{(0)}), (A^{(1)}, B^{(1)}), \dots$$

by the rule

$$A^{(k+1)} = F_k^* A^{(k)} F_k$$
,  $B^{(k+1)} = F_k^* B^{(k)} F_k$ ,  $k \ge 0$ .

Here  $F_k$  is an elementary plane matrix defined by the pivot pair (i(k), j(k))

$$F_k = \begin{bmatrix} I & & & \\ & 1 & & \alpha_k & \\ & & I & & \\ & & \beta_k & 1 & \\ & & & & I \end{bmatrix} \begin{array}{c} i(k) & & \\ i(k) & & \\ j(k) & & \\ \end{array}$$

The goal is to compute complex numbers  $\alpha_k$ ,  $\beta_k$  such that the pivot elements  $a_{ij}^{(k)}$ ,  $b_{ij}^{(k)}$  of  $A^{(k)}$ ,  $B^{(k)}$  are annihilated.

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We simplify notation:  $A = A^{(k)}, A' = A^{(k+1)}, F = F_k, (i,j) = (i(k), j(k)).$ 

Pivot submatrices  $\hat{A}$ ,  $\hat{B}$ ,  $\hat{F}$  of A, B, F are 2 × 2 principal submatrices obtained on the intersection of pivot rows and columns *i* and *j*.
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We have

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

and F is chosen to obtain  $a'_{ij} = 0$  and  $b'_{ij} = 0$ .

## Derivation of the Complex FL Method (n = 2)

The goal is to compute  $\alpha$  and  $\beta$  which satisfy the matrix equations

$$\begin{bmatrix} 1 & \bar{\beta} \\ \bar{\alpha} & 1 \end{bmatrix} \begin{bmatrix} a_{ii} & a_{ij} \\ \bar{a}_{ij} & a_{jj} \end{bmatrix} \begin{bmatrix} 1 & \alpha \\ \beta & 1 \end{bmatrix} = \begin{bmatrix} a'_{ii} & 0 \\ 0 & a'_{jj} \end{bmatrix} \\ \begin{bmatrix} 1 & \bar{\beta} \\ \bar{\alpha} & 1 \end{bmatrix} \begin{bmatrix} b_{ii} & b_{ij} \\ \bar{b}_{ij} & b_{jj} \end{bmatrix} \begin{bmatrix} 1 & \alpha \\ \beta & 1 \end{bmatrix} = \begin{bmatrix} b'_{ii} & 0 \\ 0 & b'_{jj} \end{bmatrix}.$$

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This leads us to solving a system of two nonlinear equations

$$e_1 = a_{ii}\alpha + a_{jj}\bar{\beta} + \bar{a}_{ij}\alpha\bar{\beta} + a_{ij} = 0$$
  

$$e_2 = b_{ii}\alpha + b_{jj}\bar{\beta} + \bar{b}_{ij}\alpha\bar{\beta} + b_{ij} = 0.$$

#### Solution if Matrices are Real and Symmetric

$$\begin{aligned} \Im_{ii} &= a_{ii}b_{ij} - a_{ij}b_{ii} = \begin{vmatrix} a_{ii} & b_{ii} \\ a_{ij} & b_{ij} \end{vmatrix} \\ \Im_{jj} &= a_{jj}b_{ij} - a_{ij}b_{jj} = \begin{vmatrix} a_{jj} & b_{jj} \\ a_{ij} & b_{ij} \end{vmatrix} \\ \Im_{ij} &= a_{ii}b_{jj} - a_{jj}b_{ii} = \begin{vmatrix} a_{ii} & b_{ii} \\ a_{jj} & b_{jj} \end{vmatrix} \\ \Im &= \Im_{ij}^{2} + 4\Im_{ii}\Im_{jj} \\ \nu &= (\Im_{ij} + \operatorname{sgn}(\Im_{ij})\sqrt{\Im})/2 \\ \alpha &= \Im_{j}/\nu, \quad \beta = -\Im_{i}/\nu \end{aligned}$$

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If  $\begin{bmatrix} a_{ii} & a_{ij} \\ \bar{a}_{ij} & a_{jj} \end{bmatrix}$  and  $\begin{bmatrix} b_{ii} & b_{ij} \\ \bar{b}_{ij} & b_{jj} \end{bmatrix}$  are proportional, all  $\Im_{ii}$ ,  $\Im_{jj}$ ,  $\Im_{ij}$ ,  $\Im_{ij}$ ,  $\Im$  and  $\nu$  are zero and a special algorithm is required. This is the real FL algorithm.

#### The Complex FL Algorithm

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- Difficult and challenging for making a good numerical code (to many freedoms, all we have  $\alpha A + \beta B \succ O$ , when to stop iterations?)
- Theoretical results are lacking (all we have is quadratic asymptotic convergence result)

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

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

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 $\hat{Z}$  is sought in the form of a product of two Jacobi rotations and one or two diagonal matrices.

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Both approaches yield the same algorithm.

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

$$\hat{B} \to \operatorname{diag} \qquad \hat{B} \to I_{2}$$

$$\uparrow \qquad \uparrow$$

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

$$\cdot \begin{bmatrix} \cos(\theta - \frac{\pi}{4}) & -e^{i\alpha}\sin(\theta - \frac{\pi}{4}) \\ e^{-i\alpha}\sin(\theta - \frac{\pi}{4}) & \cos(\theta - \frac{\pi}{4}) \end{bmatrix} \cdot \begin{bmatrix} e^{i\omega_{i}} & 0 \\ 0 & e^{i\omega_{j}} \end{bmatrix}$$

$$\downarrow \qquad \qquad \downarrow$$

$$\hat{A} \to \operatorname{diag} \qquad \operatorname{diag}(\hat{Z}) \succ O$$

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$$b=|b_{ij}|,\quad t=\sqrt{1-b^2},\quad e=a_{jj}-a_{ii},\quad \ \epsilon=\left\{egin{array}{cc} 1,&e\geq0\ -1,&e<0\end{array}
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 $\begin{array}{rcl} u+\imath\,v &=& e^{-\imath\,\mathrm{arg}(b_{ij})}\,a_{ij}, & \tan\gamma=2\frac{v}{e}, & -\frac{\pi}{2}<\gamma\leq\frac{\pi}{2}\\ \tan2\theta &=& \epsilon\frac{2u-(a_{ii}+a_{ji})b}{t\sqrt{e^2+4v^2}}, & -\frac{\pi}{4}<\theta\leq\frac{\pi}{4}\\ 2\cos^2\phi &=& 1+b\sin2\theta+t\cos2\theta\cos\gamma, & 0\leq\phi\leq\frac{\pi}{2}\\ 2\cos^2\psi &=& 1-b\sin2\theta+t\cos2\theta\cos\gamma, & 0\leq\psi\leq\frac{\pi}{2}\\ e^{\imath\alpha}\sin\phi &=& \frac{e^{\imath\,\mathrm{arg}(b_{ij})}}{2\cos\psi}\left[\sin2\theta-b-\imath t\cos2\theta\sin\gamma\right]\\ e^{-\imath\beta}\sin\psi &=& \frac{e^{-\imath\,\mathrm{arg}(b_{ij})}}{2\cos\phi}\left[\sin2\theta+b+\imath t\cos2\theta\sin\gamma\right]. \end{array}$ 

Then

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

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## Derivation of Complex CJ Method, $B \succ O$

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- The real CJ algorithm is obtained by simplifying the complex one

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

$$\left[\begin{array}{cc}1 & b_{ij}\\ \bar{b}_{ij} & 1\end{array}\right] = \hat{B} = \hat{L}\hat{L}^* = \left[\begin{array}{cc}1 & 0\\ \bar{a} & \bar{c}\end{array}\right] \left[\begin{array}{cc}1 & a\\ 0 & c\end{array}\right] = \left[\begin{array}{cc}1 & a\\ \bar{a} & |a|^2 + |c|^2\end{array}\right]$$

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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
$$\begin{bmatrix} -2i & -2i \\ 0 & 1 \end{bmatrix} = \frac{2i}{\tau} \begin{bmatrix} 2i & -b_{ij} \\ 0 & 1 \end{bmatrix}$$

$$\hat{F}_{1}^{*}\hat{A}\hat{F}_{1} = \left[egin{array}{cc} a_{ii} & (a_{ij} - b_{ij}a_{ii})/ au\ (ar{a}_{ij} - ar{b}_{ij}a_{ii})/ au\ (ar{a}_{ij} - ar{b}_{ij}a_{ii})/ au\ (ar{a}_{jj} - ar{b}_{ij}a_{ii})/ au\ (ar{a}_{jj} - ar{b}_{ij}a_{ii})|b_{ij}|^{2}\ (ar{a}_{ij} - ar{b}_{ij}a_{ij})|b_{ij}|^{2}\ (ar{b}_{ij}a_{ij})|b_{ij}|^{2}\ (ar{b}_{ij}a_{ij})|b_{ij}|^{2}\ (ar{b}_{ij}a_{ij}a_{ij})|b_{ij}|^{2}\ (ar{b}_{ij}a_{ij$$

.

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 that the (1,2)-element of  $\hat{R}_1$  is  $-e^{i\epsilon_1} \sin \vartheta_1$ . Then the angles  $\vartheta_1$  and  $\epsilon_1$  are determined by the formulas

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

The transformation formulas for the diagonal elements of A read

$$\begin{array}{lll} a'_{ii} & = & a_{ii} + \tan \vartheta_1 \cdot \frac{|a_{ij} - a_{ii}b_{ij}|}{\sqrt{1 - b_{ij}^2}} \\ a'_{jj} & = & a_{jj} - \frac{a_{ij}\bar{b}_{ij} + \bar{a}_{ij}b_{ij} - (a_{ii} + a_{jj})|b_{ij}|^2}{1 - |b_{ij}|^2} - \tan \vartheta_1 \cdot \frac{|a_{ij} - a_{ii}b_{ij}|}{\sqrt{1 - b_{ij}^2}}. \end{array}$$

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

Let 
$$c_{\vartheta_1} = \cos \vartheta_1$$
,  $s_{\vartheta_1}^{\pm} = e^{\pm i\epsilon_1} \sin \vartheta_1$ . Then  

$$\hat{F} = \frac{1}{\sqrt{1 - |b_{ij}|^2}} \begin{bmatrix} \sqrt{1 - |b_{ij}|^2} & -b_{ij} \\ 0 & 1 \end{bmatrix} \begin{bmatrix} c_{\vartheta_1} & -s_{\vartheta_1}^+ \\ s_{\vartheta_1}^- & c_{\vartheta_1} \end{bmatrix}$$

$$= \frac{1}{\sqrt{1 - |b_{ij}|^2}} \begin{bmatrix} c_{\vartheta_1} & -s_{\vartheta_1} \\ s_{\vartheta_1}^- & c_{\vartheta_1} \end{bmatrix}$$
 $c_{\vartheta_1} = c_{\vartheta_1}\sqrt{1 - |b_{ij}|^2} - s_{\vartheta_1}^- b_{ij}$ 
 $s_{\vartheta_1} = c_{\vartheta_1}b_{ij} + s_{\vartheta_1}^+\sqrt{1 - |b_{ij}|^2}$ 
 $= \begin{bmatrix} c_1 & -s_1 \\ s_2 & c_2 \end{bmatrix},$ 
 $c_1 = c_{\vartheta_1} - s_{\vartheta_1}^- b_{ij}/\sqrt{1 - |b_{ij}|^2}, \quad c_2 = c_{\vartheta_1}/\sqrt{1 - |b_{ij}|^2},$ 
 $s_1 = c_{\vartheta_1}b_{ij}/\sqrt{1 - |b_{ij}|^2} + s_{\vartheta_1}^+, \quad s_2 = s_{\vartheta_1}^-/\sqrt{1 - |b_{ij}|^2}.$ 

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Assuming positive c, one obtains  $a = b_{ij}$ ,  $c = \sqrt{1 - |b_{ij}|^2} = \tau$ . Hence

$$\hat{R} = \left[ egin{array}{cc} au & b_{ij} \\ 0 & 1 \end{array} 
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ight].$$

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 Algorithm *RR*\**J*

$$\hat{F}_{2}^{*}\hat{A}\hat{F}_{2}=\left[egin{array}{cc} a_{ii}-rac{a_{ij}ar{b}_{ij}+ar{a}_{ij}b_{ij}-(a_{ii}+a_{jj})|b_{ij}|^{2}}{ au^{2}}&(a_{ij}-a_{jj}b_{ij})/ au\ &(a_{ij}-a_{jj}b_{ij})/ au\end{array}
ight]$$

• The final transformation is  $\hat{F} = \hat{F}_2 \hat{R}_2$ ,

- $\hat{R}_2$  is the Jacobi rotation which annihilates (1,2)-element of  $\hat{F}_2^*\hat{A}\hat{F}_2$
- Let (1,2)-element of  $\hat{R}_2$  be  $-e^{\imath\epsilon_2}\sin\vartheta_2$

Then the parameters  $\epsilon_2$  and  $\vartheta_2$  are determined by the formulas

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

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If  $a_{ii} = a_{jj}$ ,  $a_{ij} = a_{jj}b_{ij}$ ,  $\vartheta_2$  is not well defined and we choose  $\vartheta_2 = 0$ . In that case  $a'_{ii}$  and  $a'_{jj}$  reduce to  $a_{ii}$  and  $a_{jj}$ , respectively.

## The Algorithm RR\*J

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et 
$$c_{\vartheta_2} = \cos \vartheta_2$$
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$$\hat{F} = \frac{1}{\sqrt{1 - |b_{ij}|^2}} \begin{bmatrix} 1 & 0\\ -\bar{b}_{ij} & \sqrt{1 - |b_{ij}|^2} \end{bmatrix} \begin{bmatrix} c_{\vartheta_2} & -s_{\vartheta_2}^+\\ s_{\vartheta_2}^- & c_{\vartheta_2} \end{bmatrix}$$

$$= \frac{1}{\sqrt{1 - |b_{ij}|^2}} \begin{bmatrix} c_{\vartheta_2} & -s_{\vartheta_2}^+\\ s_{\vartheta_2}^- & c_{\vartheta_2}^- \end{bmatrix}, \quad c_{\vartheta_2}^- = c_{\vartheta_2}\sqrt{1 - |b_{ij}|^2} + s_{\vartheta_2}^+ \bar{b}_{ij}$$

$$= \begin{bmatrix} c_1 & -s_1\\ s_2 & c_2 \end{bmatrix}, \quad \text{It is easy to check that } c_{\vartheta}^2 + s_{\vartheta}^2 = 1.$$

$$egin{aligned} c1 &= c_{artheta_2}/\sqrt{1-b_{ij}^2}, & c2 &= c_{artheta_2}+s_{artheta_2}^+ar{b}_{ij}/\sqrt{1-b_{ij}^2}, \ s1 &= s_{artheta_2}^+/\sqrt{1-b_{ij}^2}^+, & s2 &= s_{artheta_2}^--c_{artheta_2}ar{b}_{ij}/\sqrt{1-b_{ij}^2}. \end{aligned}$$

We can postmultiply  $\hat{F}$  by 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 CJ is a hybrid algorithm which can be briefly defined as follows:
select the pivot pair (i, j)

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

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$$A_{\mathcal{S}} = [\mathsf{diag}(A)]^{-1/2} A[\mathsf{diag}(A)]^{-1/2}, \quad B_{\mathcal{S}} = [\mathsf{diag}(B)]^{-1/2} B[\mathsf{diag}(B)]^{-1/2}$$

$$\varrho_{(A,B)} = \max_{1 \le i \le n} \frac{|\tilde{\lambda}_i - \lambda_i|}{\lambda_i} / \sqrt{\kappa_2^2(A_S) + \kappa_2^2(B_S)}$$

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

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

## Relative errors: CFL vs. MATLAB eig(A,B)


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