KU LEUVEN

Pole swapping methods for the eigenvalue problem

Rational QR algorithms

Daan Camps

9/6/19
Berkeley Lab Seminar

KU Leuven - University of Leuven - Department of Computer Science - NUMA Section

Acknowledgements

Collaborators:

- Raf Vandebril
- Karl Meerbergen
- Paul Van Dooren
- Thomas Mach
- David Watkins
- Nicola Mastronardi

Overview

Introduction

Generalized eigenvalue problems

- Let $A, B \in \mathbb{F}^{n \times n}$ determine a *matrix pair* (A, B) or *matrix pencil* $A - \lambda B$.

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- Regularity: n eigenvalues (counting multiplicities) including infinite eigenvalues (singular B)

Generalized eigenvalue problems: generalized (real) Schur decomposition

- For $A - \lambda B$ with $A, B \in \mathbb{F}^{n \times n}$ there exists unitary Q and Z such that

$$Q^*(A - \lambda B)Z = S - \lambda T$$

with $S - \lambda T$ upper triangular and $\Lambda(A, B) = \{s_{11}/t_{11}, s_{22}/t_{22}, \ldots\}$.

Generalized Schur decomposition of $A - \lambda B$.

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- For $A - \lambda B$ with $A, B \in \mathbb{R}^{n \times n}$ there exists orthonormal Q and Z such that

$$Q^T(A, B)Z = (S, T) = \left(\begin{bmatrix} S_{11} & S_{12} & \ldots & S_{1m} \\ 0 & S_{22} & \ddots & S_{2m} \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \ldots & 0 & S_{mm} \end{bmatrix}, \begin{bmatrix} T_{11} & T_{12} & \ldots & T_{1m} \\ 0 & T_{22} & \ddots & T_{2m} \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \ldots & 0 & T_{mm} \end{bmatrix} \right),$$

where (S_{ii}, T_{ii}), $i = 1, \ldots, m$ of dimension 1×1 or 2×2.

Generalized real Schur decomposition of $A - \lambda B$.

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- Listed in *"Top Ten Algorithms of the Century."* by Computing in Science and Engineering (2000)

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  2. Iterative bulge chasing phase to compute (real) generalized Schur decomposition

$$S - \lambda T = Q^*(A - \lambda B)Z$$

Bulge chasing

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$$A - \lambda B$$

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$$Q_1^*(A - \lambda B)Z_1$$

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$$Q_2^* Q_1^* (A - \lambda B) Z_1$$

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Bulge chasing

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  $\Rightarrow$ iterates are uniquely determined by $\boldsymbol{q}_1 = p(AB^{-1})\boldsymbol{e}_1$ and thus by *shifts*.

Bulge chasing

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$\rightarrow$ These results are based on a connection with Krylov subspaces.

Pole swapping

Rational QZ

Hessenberg pencils

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Rational QZ

Hessenberg pencils

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Rational QZ

Hessenberg pencils

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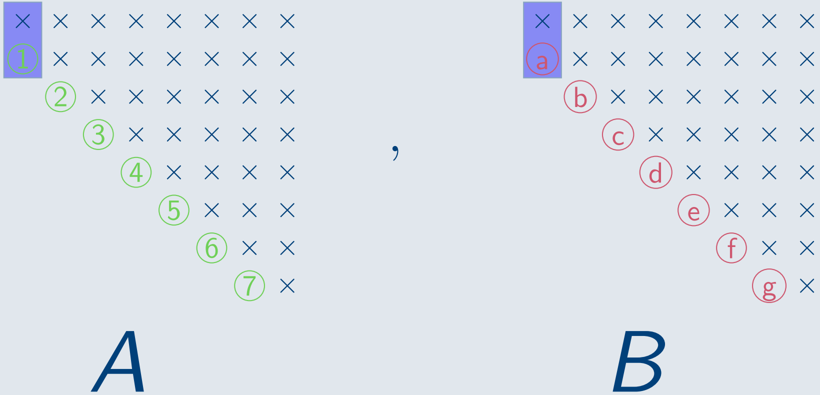
 & \textcircled{b} & \times & \times & \times & \times & \times & \times \\
 & & \textcircled{c} & \times & \times & \times & \times & \times \\
 & & & \textcircled{d} & \times & \times & \times & \times \\
 & & & & \textcircled{e} & \times & \times & \times \\
 & & & & & \textcircled{f} & \times & \times \\
 & & & & & & \textcircled{g} & \times
\end{matrix}}_{B}
$$

pole tuple $\Xi = \left(\frac{\textcircled{1}}{\textcircled{a}}, \frac{\textcircled{2}}{\textcircled{b}}, \ldots\right) \subset \bar{\mathbb{C}}$

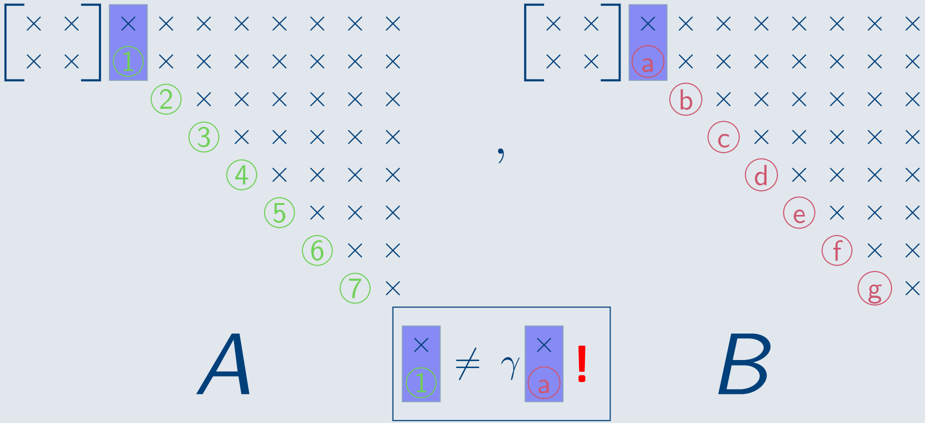
Rational QZ: an example

Introducing a shift

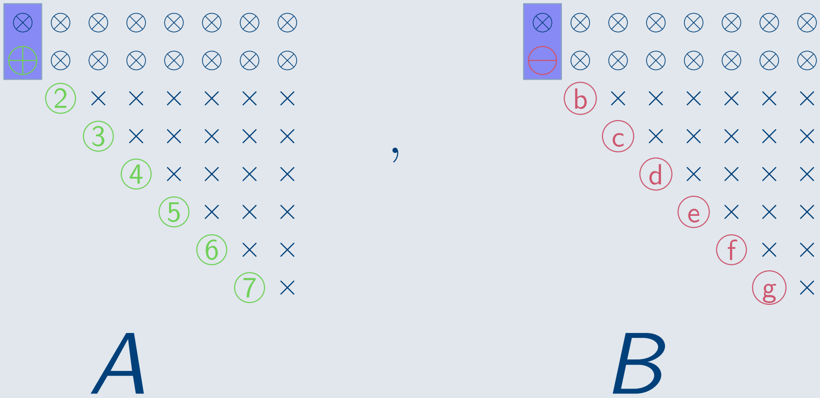


Rational QZ: an example

Introducing a shift



Introducing a shift



Rational QZ: an example

Introducing a shift

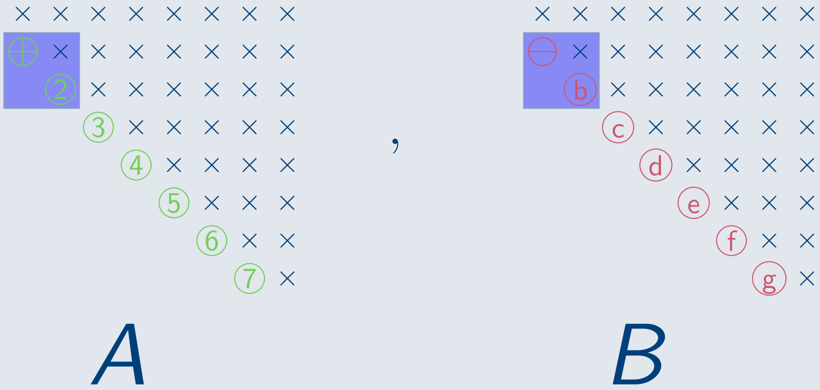
- $A, B \in \mathbb{C}^{n\times n}$ Hessenberg with poles $\Xi = (\xi_1, \dots, \xi_{n-1})$
- Change ξ_1 to another pole $\hat{\xi}_1$:
  - $\boldsymbol{x} = \gamma\,(A - \hat{\xi}_1 B)(A - \xi_1 B)^{-1}\boldsymbol{e}_1 = \hat{\gamma}(A - \hat{\xi}_1 B)\boldsymbol{e}_1,$
  - $Q_1^* \boldsymbol{x} = \alpha \boldsymbol{e}_1,$
- $\hat{A} - \lambda \hat{B} = Q_1^*(A - \lambda B)$

$$(\hat{A} - \hat{\xi}_1 \hat{B})\boldsymbol{e}_1 = Q_1^*(A - \hat{\xi}_1 B)\boldsymbol{e}_1 = \tilde{\gamma} Q_1^* \boldsymbol{x} = \alpha\,\tilde{\gamma}\boldsymbol{e}_1$$

- One exception: $(A - \xi_1 B)\boldsymbol{e}_1 = \boldsymbol{0}$

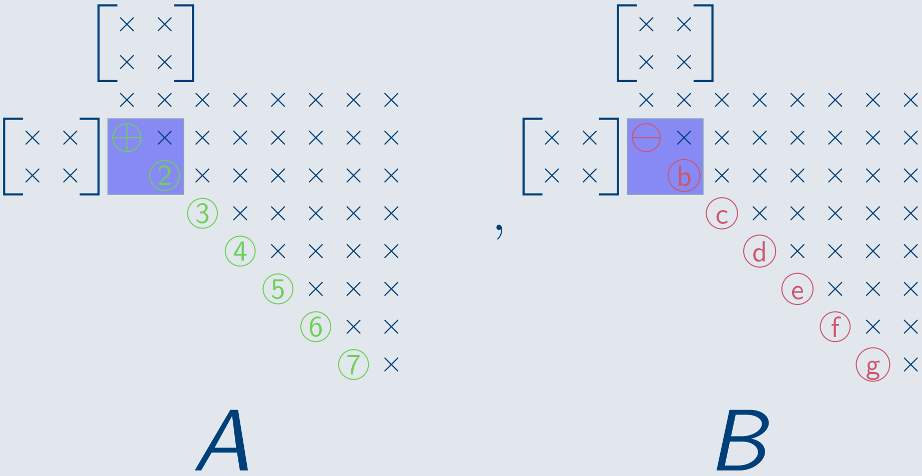
Rational QZ: an example

Swapping poles



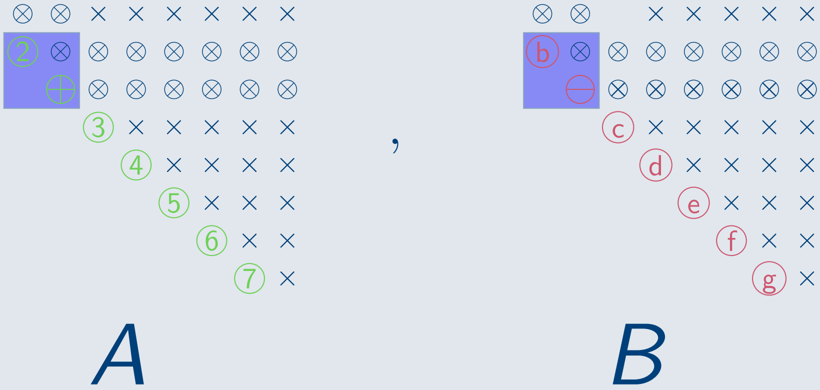
Rational QZ: an example

Swapping poles



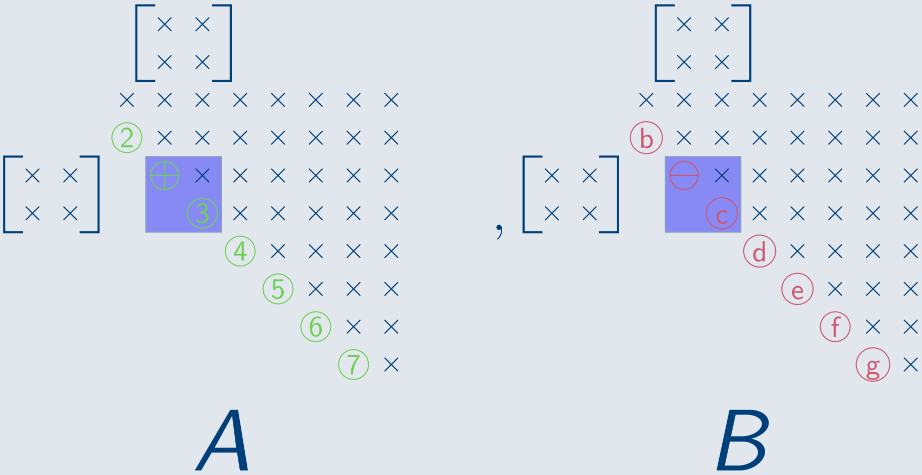
Rational QZ: an example

Swapping poles



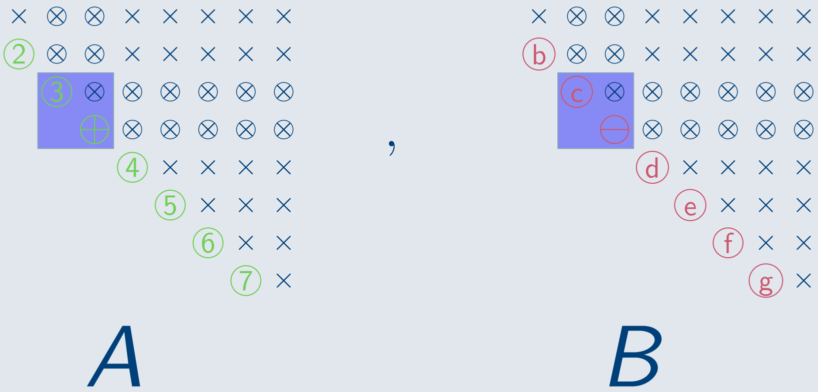
Rational QZ: an example

Swapping poles



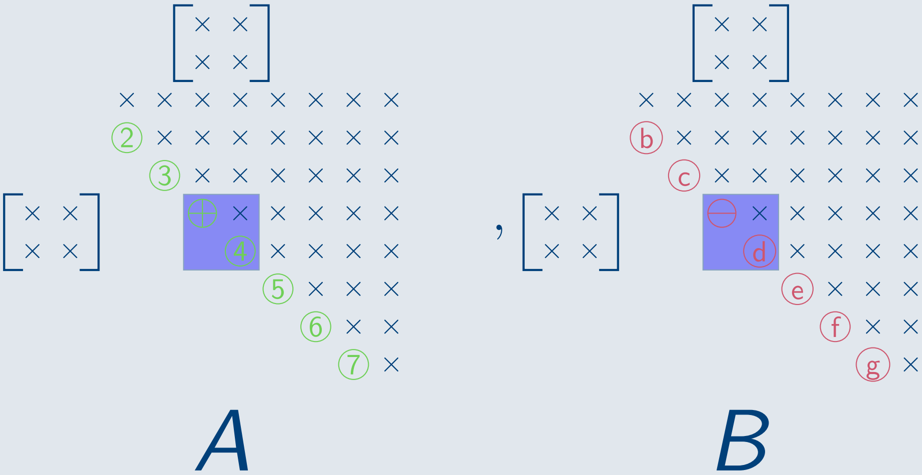
Rational QZ: an example

Swapping poles



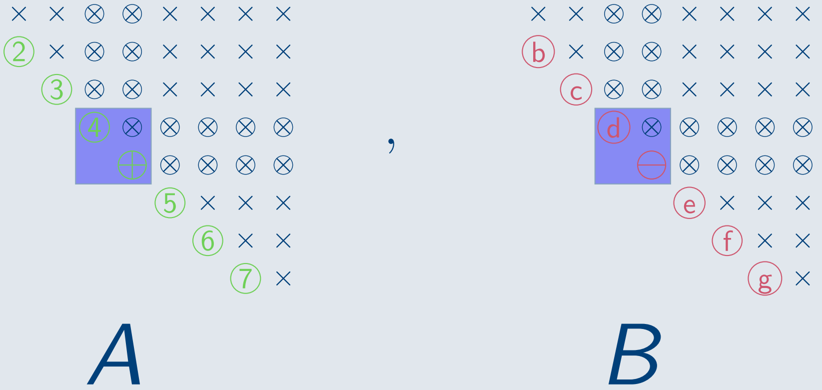
Rational QZ: an example

Swapping poles



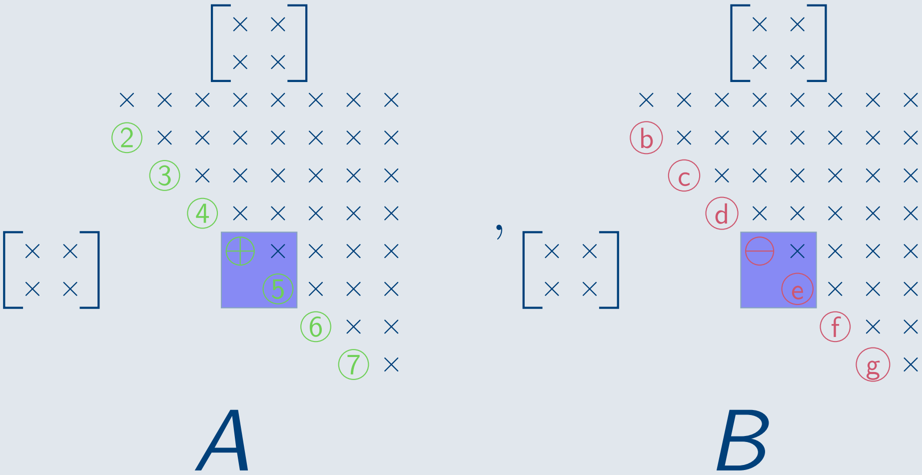
Rational QZ: an example

Swapping poles



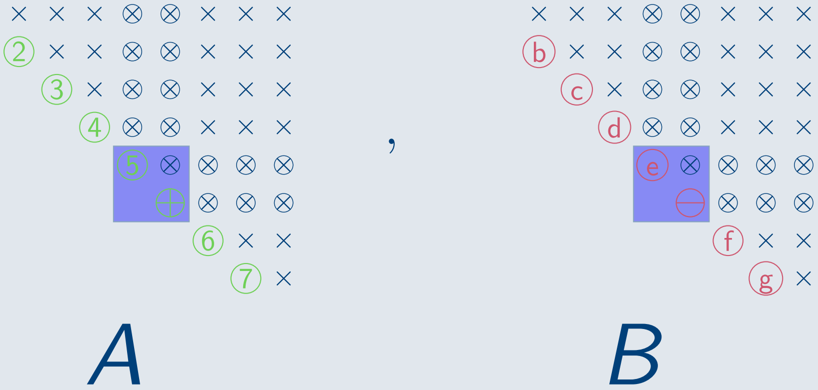
Rational QZ: an example

Swapping poles



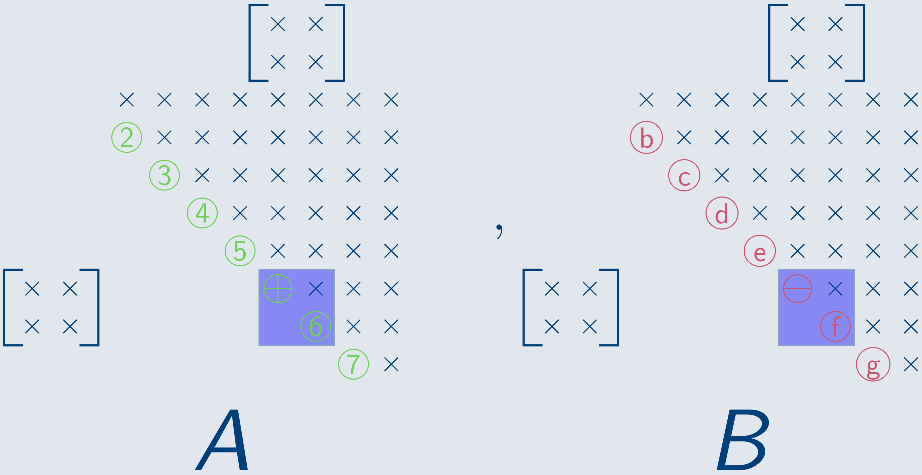
Rational QZ: an example

Swapping poles



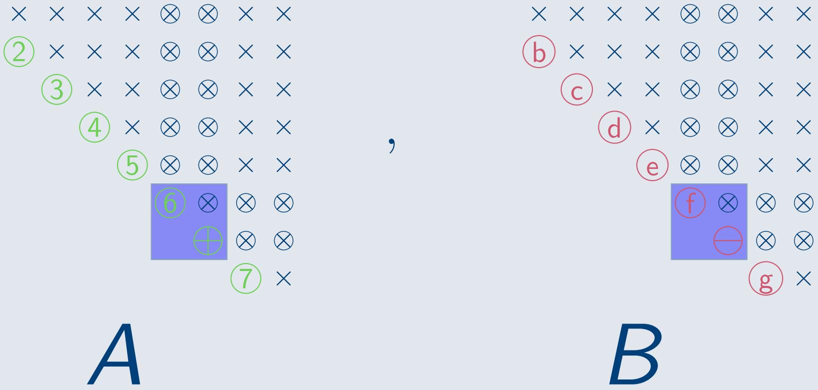
Rational QZ: an example

Swapping poles



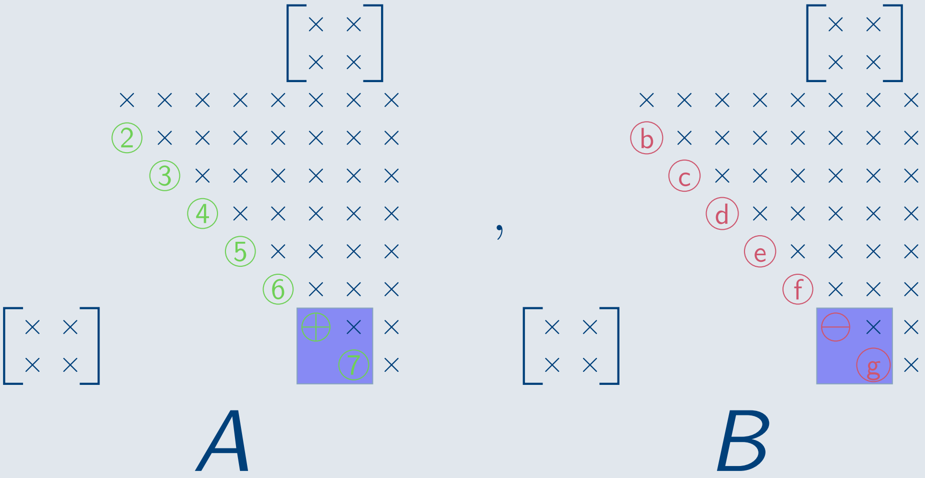
Rational QZ: an example

Swapping poles



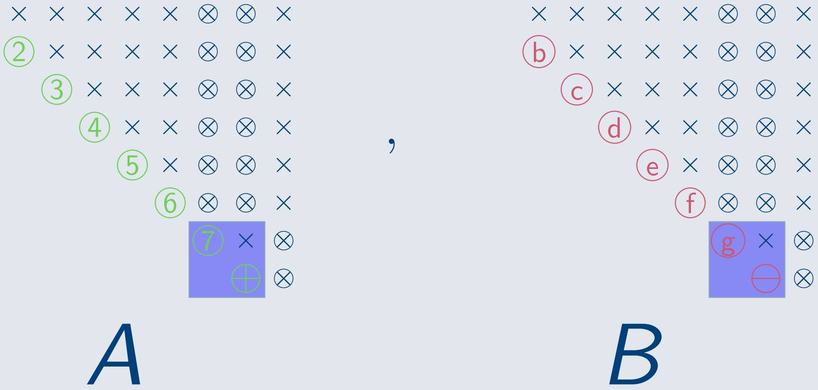
Rational QZ: an example

Swapping poles



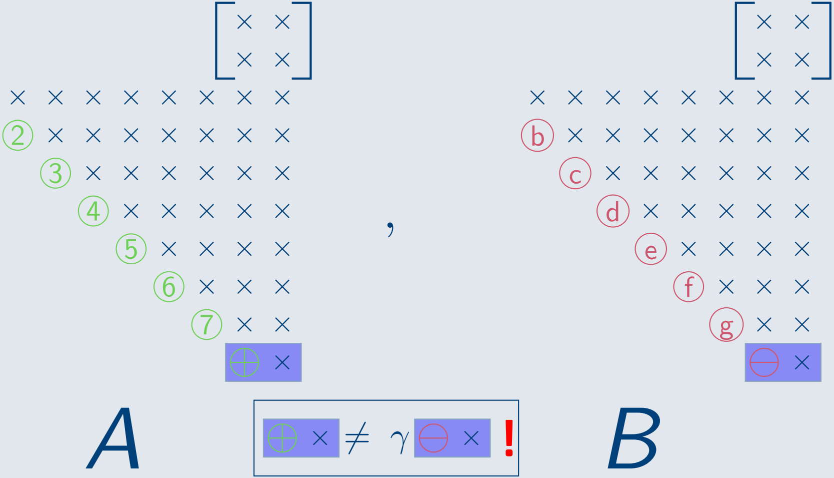
Rational QZ: an example

Swapping poles



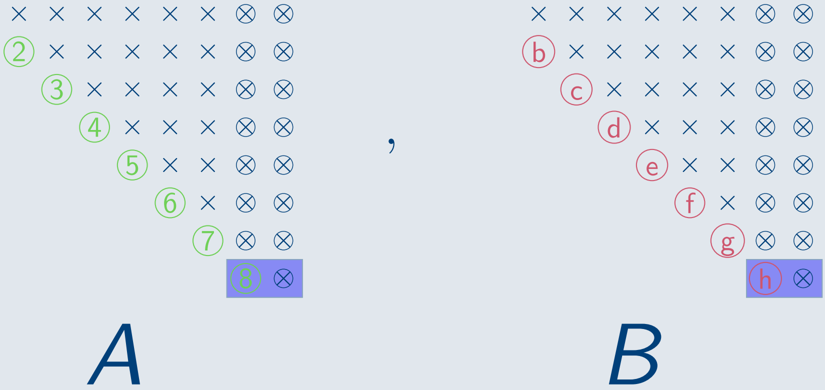
Rational QZ: an example

Introducing a pole



Rational QZ: an example

Introducing a pole



Classical QZ as a special case

$$
\underset{A}{\begin{matrix}
\times & \times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times & \times \\
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 & & & & & \times & \times & \times \\
 & & & & & & \times & \times
\end{matrix}}
,
\underset{B}{\begin{matrix}
\times & \times & \times & \times & \times & \times & \times & \times \\
 & \times & \times & \times & \times & \times & \times & \times \\
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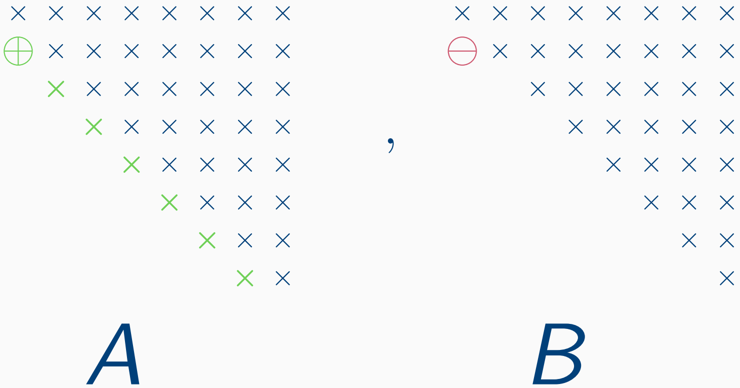
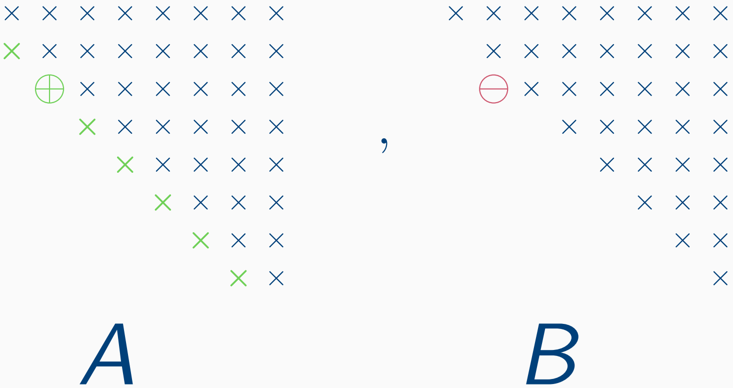
 & & & & & & & \times
\end{matrix}}
$$

Classical QZ as a special case



Classical QZ as a special case



Computing the swap: problem statement

We want to compute:

$$Q^*(A - \lambda B)Z = Q^* \left(\begin{bmatrix} \alpha_1 & a \\ & \alpha_2 \end{bmatrix} - \lambda \begin{bmatrix} \beta_1 & b \\ & \beta_2 \end{bmatrix} \right) Z = \begin{bmatrix} \hat{\alpha}_1 & \hat{a} \\ & \hat{\alpha}_2 \end{bmatrix} - \lambda \begin{bmatrix} \hat{\beta}_1 & \hat{b} \\ & \hat{\beta}_2 \end{bmatrix} = \hat{A} - \lambda \hat{B},$$

with:

- $\alpha_1/\beta_1 = \hat{\alpha}_2/\hat{\beta}_2 = \xi_1$
- $\alpha_2/\beta_2 = \hat{\alpha}_1/\hat{\beta}_1 = \xi_2$

Classical problem in NLA:

- Van Dooren (1981)
- Kågström (1993)
- C.-Mach-Vandebril-Watkins (2019)

Computing the swap: problem statement

We need to construct $Z = [\boldsymbol{z}_1 \ \boldsymbol{z}_2]$, $Q = [\boldsymbol{q}_1 \ \boldsymbol{q}_2]$ in such a way that:

- $\boldsymbol{q}_1$, $\boldsymbol{z}_1$ are a *deflating pair* for $A - \lambda B$ corresponding to the eigenvalue ξ_2, i.e.

$$(A - \lambda B)\boldsymbol{z}_1 = \gamma_1 \boldsymbol{q}_1(\alpha_2 - \lambda\beta_2),$$

- similarly, $\boldsymbol{q}_2$, $\boldsymbol{z}_2$ are a deflating pair for ξ_1,

$$(A - \lambda B)\boldsymbol{z}_2 = \gamma_2 \boldsymbol{q}_2(\alpha_1 - \lambda\beta_1).$$

It then follows from the orthogonality of Q, Z that

$$\boldsymbol{q}_2^* A \boldsymbol{z}_1 = \boldsymbol{q}_2^* B \boldsymbol{z}_1 = 0,$$

and thus the swapping is achieved.

Computing the swap: two methods

Two options:

- **1. First Z, then Q:**

$$H_1 = \beta_2 A - \alpha_2 B = \begin{bmatrix} \times & \times \\ 0 & 0 \end{bmatrix}$$

$$H_1 Z = (\beta_2 A - \alpha_2 B) Z = \begin{bmatrix} 0 & \times \\ 0 & 0 \end{bmatrix}$$

$\Rightarrow$ $\boldsymbol{z}_1$ is a right eigenvector of $A - \lambda B$ associated with ξ_2

$\Rightarrow$ $A\boldsymbol{z}_1$ and $B\boldsymbol{z}_1$ are parallel, rotation Q can simultaneously introduce a zero in position $(2, 1)$ of both AZ and BZ

Computing the swap: two methods

Two options:

- **2. First Q, then Z:**

$$H_2 = \beta_1 A - \alpha_1 B = \begin{bmatrix} 0 & \times \\ 0 & \times \end{bmatrix}$$

$$Q^* H_2 = Q^*(\beta_1 A - \alpha_1 B) = \begin{bmatrix} 0 & \times \\ 0 & 0 \end{bmatrix}$$

$\Rightarrow$ $\boldsymbol{q}_2^*$ is a left eigenvector of $A - \lambda B$ associated with ξ_1

$\Rightarrow$ $\boldsymbol{q}_2^* A$ and $\boldsymbol{q}_2^* B$ are parallel,rotation Z can simultaneously introduce a zero in position $(2,1)$ of $Q^* A$ and $Q^* B$

Computing the swap: finite precision

Theorem C.-Mach-Vandebril-Watkins (2019)

Let

$$A - \lambda B = \begin{bmatrix} \alpha_1 & a \\ & \alpha_2 \end{bmatrix} - \lambda \begin{bmatrix} \beta_1 & b \\ & \beta_2 \end{bmatrix},$$

with $\alpha_1/\beta_1 = \xi_1$, and $\alpha_2/\beta_2 = \xi_2$. Furthermore, assume $|\xi_1| \geq |\xi_2|$. If the swapping is computed by first deriving $\tilde{Z}$, as described in method 1 above, and afterwards computing $\tilde{Q}$ such that $Q^*(BZ\boldsymbol{e}_1) = \gamma \boldsymbol{e}_1$, then we have that the computed transformations satisfy:

$$\tilde{Q}^*(A + E_A, B + E_B)\tilde{Z} = \left(\begin{bmatrix} \tilde{\alpha}_1 & \tilde{a} \\ & \tilde{\alpha}_2 \end{bmatrix}, \begin{bmatrix} \tilde{\beta}_1 & \tilde{b} \\ & \tilde{\beta}_2 \end{bmatrix} \right),$$

with $\|E_A\|_2 \leq c\epsilon_m \|A\|_2$, $\|E_B\|_2 \leq c\epsilon_m \|B\|_2$, c a small constant.

Computing the swap: finite precision

Table 1: Numerical methods to compute a backward stable pole swap.

$\lvert\xi_1\rvert \geq \lvert\xi_2\rvert$	$\lvert\xi_1\rvert < \lvert\xi_2\rvert$
1.A) First Z, then Q from $Q^*(BZ\boldsymbol{e}_1) = \gamma \boldsymbol{e}_1$	1.B) First Z, then Q from $Q^*(AZ\boldsymbol{e}_1) = \gamma \boldsymbol{e}_1$
2.A) First Q, then Z from $(\boldsymbol{e}_2^* Q^* A)Z = \gamma \boldsymbol{e}_2^*$	2.B) First Q, then Z from $(\boldsymbol{e}_2^* Q^* B)Z = \gamma \boldsymbol{e}_2^*$

Computing the swap: numerics

Table 2: Distribution of errors $|\hat{a}_{21}|/\|A\|$ and $|\hat{b}_{21}|/\|B\|$ for our method, Van Dooren's method, and the Sylvester method.

$\lvert\hat{x}_{21}\rvert/\|X\|$		$[0, 10^{-16}]$	$(10^{-16}, 10^{-15}]$	$(10^{-15}, 10^{-10}]$	$(10^{-10}, 10^{-5}]$	$(10^{-5}, 10^{0}]$
Our method	A	99.71%	0.29%	0%	0%	0%
	B	99.85%	0.15%	0%	0%	0%
Van Dooren	A	98.19%	0.55%	0.93%	0.27%	0.06%
	B	98.19%	0.55%	0.93%	0.27%	0.06%
Sylvester	A	93.34%	5.88%	0.57%	0.17%	0.04%
	B	93.34%	5.88%	0.57%	0.17%	0.04%

Rational Krylov Matrices and Subspaces

- **Krylov subspace**

$$\mathcal{K}_{m+1}(A, \boldsymbol{v}) := \mathcal{R}(\boldsymbol{v}, A\boldsymbol{v}, \ldots, A^m\boldsymbol{v})$$

- **rational Krylov subspace**

$$\mathcal{K}^{\text{rat}}_{m+1}(A, \boldsymbol{v}, \Xi) := q(A)^{-1}\mathcal{K}_{m+1}(A, \boldsymbol{v})$$

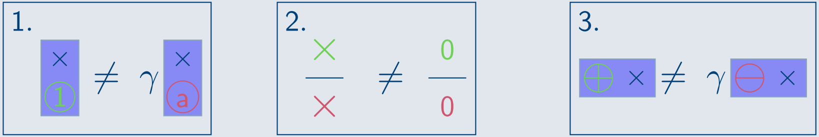
$$\Xi = (\xi_1, \ldots, \xi_m) \subset \bar{\mathbb{C}} \setminus \Lambda, \qquad q(z) = \textstyle\prod_{\xi_i \neq \infty}(z - \xi_i)$$

- **rational Krylov matrix**

$$K^{\text{rat}}_{m+1}(A, \boldsymbol{v}, \Xi) = q(A)^{-1}\left[\boldsymbol{v},\ A\boldsymbol{v},\ \ldots,\ A^m\boldsymbol{v}\right]$$

Definition: Properness.

The Hessenberg pair (A, B) is called *proper* if:



Theoretical results

Theorem (C.-Meerbergen-Vandebril, 2019a)

If (A, B) is a proper Hessenberg pair with poles $(\xi_1, \ldots, \xi_{n-1})$ distinct from the eigenvalues. Then for $i = 1, \ldots, n$:

$$\mathcal{K}_i^{\text{rat}}(AB^{-1}, \boldsymbol{e}_1, (\xi_1, \ldots, \xi_{i-1})) = \mathcal{E}_i := \mathcal{R}(\boldsymbol{e}_1, \ldots, \boldsymbol{e}_i),$$

while for $i = 1, \ldots, n-1$:

$$\mathcal{K}_i^{\text{rat}}(B^{-1}A, \boldsymbol{e}_1, (\xi_2, \ldots, \xi_i)) = \mathcal{E}_i.$$

Theoretical results

Corollary (C.-Meerbergen-Vandebril, 2019a)

If (A, B) is a proper Hessenberg pair with poles $(\xi_1, \ldots, \xi_{n-1})$ distinct from the eigenvalues. Then for $i = 1, \ldots, n$:

$$K_i^{\text{rat}}(AB^{-1}, \boldsymbol{e}_1, (\xi_1, \ldots, \xi_{i-1})) = R_i,$$

while for $i = 1, \ldots, n-1$:

$$K_i^{\text{rat}}(B^{-1}A, \boldsymbol{e}_1, (\xi_2, \ldots, \xi_i)) = \hat{R}_i.$$

Theoretical results

Implicit Q Theorem. (C.-Meerbergen-Vandebril, 2019a)

Given a regular matrix pair (A, B). The matrices Q and Z that transform it to proper Hessenberg form,

$$(\hat{A}, \hat{B}) = Q^* \, (A, B) \, Z,$$

are determined *essentially unique* if $Q\boldsymbol{e}_1$ and the (order of the) poles are fixed.

Theoretical results

Rational accelerated subspace iteration. (C.-Meerbergen-Vandebril, 2019a)

A rational QZ step with shift $\varrho \notin \{\Lambda, \Xi\}$ on a proper Hessenberg pencil with poles $(\xi_1, \ldots, \xi_{n-1})$ and new pole ξ_n, all distinct from Λ, performs nested subspace iteration for $i = 1, \ldots, n{-}1$ accelerated by

$$Q\mathcal{E}_i = \mathcal{R}(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_i) = (A - \varrho B)(A - \xi_i B)^{-1}\mathcal{E}_i$$
$$Z\mathcal{E}_i = \mathcal{R}(\boldsymbol{z}_1, \ldots, \boldsymbol{z}_i) = (A - \xi_{i+1} B)^{-1}(A - \varrho B)\mathcal{E}_i,$$

followed by a change of basis.

→ Subspace iteration with rational filter

→ More modular (single swap) convergence theory: (C.-Mach-Vandebril-Watkins, 2019).

Theoretical results

Exactness result (C., 2019)

Let (A, B) be a proper Hessenberg pencil with poles Ξ. Furthermore, let ϱ be an eigenvalue of (A, B) which is distinct from Ξ. A rational QZ step, $Q^*(A, B)Z$, with shift ϱ leads to a deflation in the last rows of $Q^*(A, B)Z$.

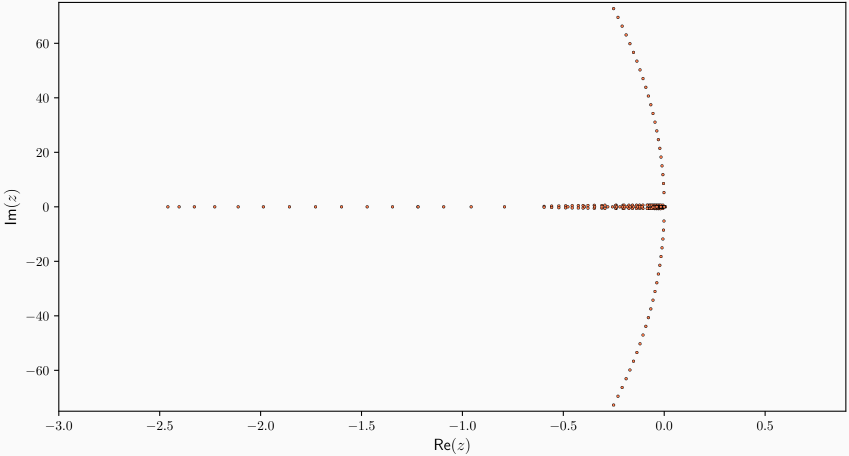
Rational QZ

Pole swapping =

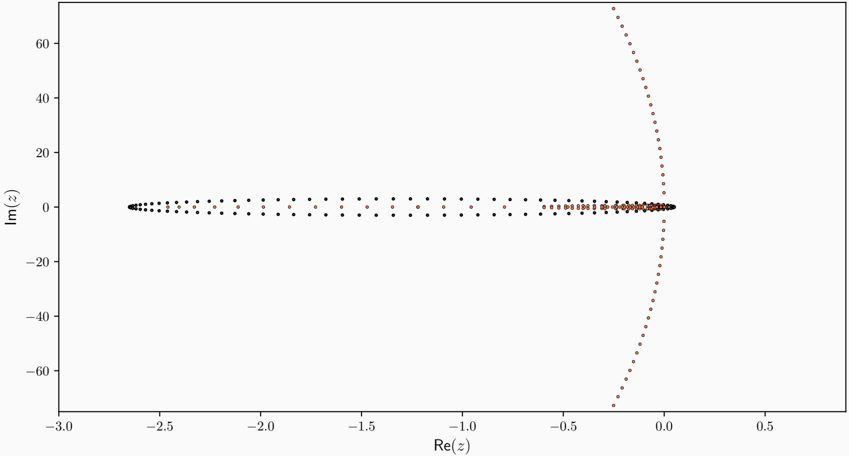
- Motivated by implicit Q theorems
  $\Rightarrow$ iterates are uniquely determined by $\boldsymbol{q}_1 = q(AB^{-1})\boldsymbol{e}_1$ and poles in pencil
- Nested subspace iteration with a change of basis accelerated by rational functions (shifts and poles)

$\rightarrow$ These results are based on a connection with rational Krylov subspaces

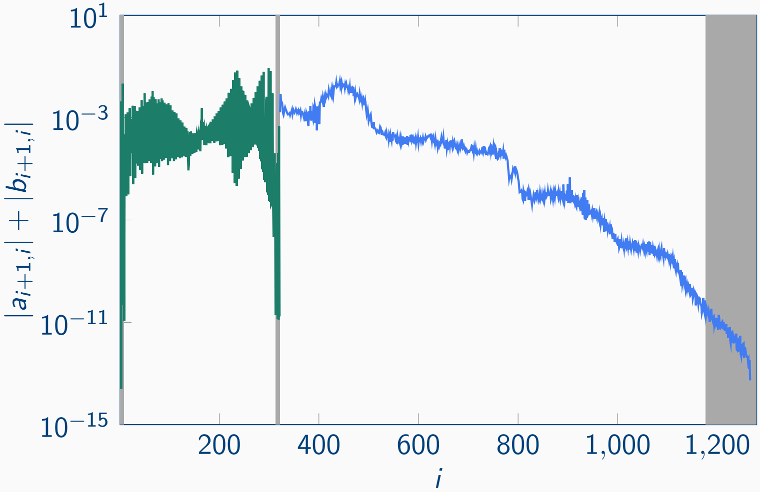
Example from Magnetohydrodynamics



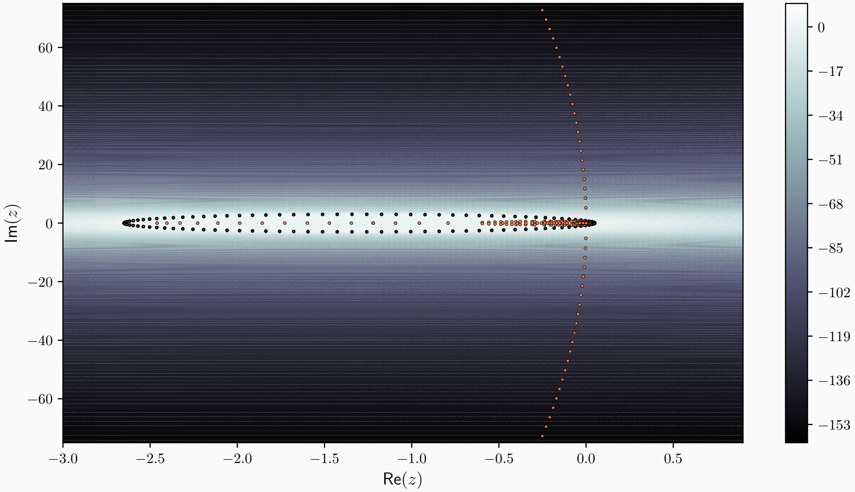
Example from Magnetohydrodynamics



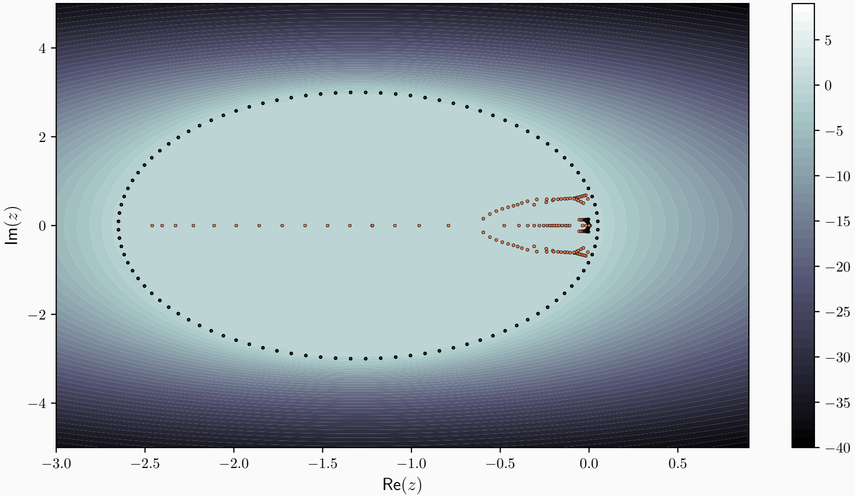
Example from Magnetohydrodynamics



Example from Magnetohydrodynamics



Example from Magnetohydrodynamics



Blocked pole swapping

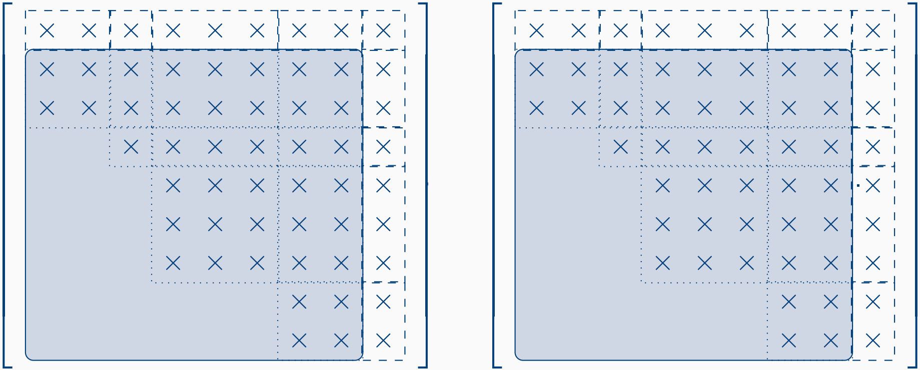
Multishift, multipole rational QZ

Motivation: make the rational QZ method competitive with state-of-the-art.

- Extension of the rational QZ method from Hessenberg to block Hessenberg pencils
- Shifts and poles of larger multiplicity
- Real-valued generalized eigenproblems in real arithmetic
- Swapping 2×2 blocks: Iterative refinement via Newton steps
- Blocked operations for improved cache usage
- Aggressive early deflation

Multishift, multipole swapping methods

Block Hessenberg pencils:



Pole pencil

Swapping 2×2 blocks

- with 1×1: similar to 1 with 1, backward stable (in practice, no error analysis yet)
- with 2×2: (Kågström, 1993)

$$Q^T \left(\begin{bmatrix} A_{11} & A_{12} \\ & A_{22} \end{bmatrix}, \begin{bmatrix} B_{11} & B_{12} \\ & B_{22} \end{bmatrix} \right) Z = \left(\begin{bmatrix} \hat{A}_{11} & \hat{A}_{12} \\ & \hat{A}_{22} \end{bmatrix}, \begin{bmatrix} \hat{B}_{11} & \hat{B}_{12} \\ & \hat{B}_{22} \end{bmatrix} \right), \qquad (1)$$

with blocks (A_{11}, B_{11}), $(\hat{A}_{22}, \hat{B}_{22})$ of dimension n_1 and blocks (A_{22}, B_{22}), $(\hat{A}_{11}, \hat{B}_{11})$ of dimension n_2. Furthermore, we require:

$$\begin{cases} \Lambda(A_{11}, B_{11}) = \Lambda(\hat{A}_{22}, \hat{B}_{22}) = \Xi^1 \\ \Lambda(A_{22}, B_{22}) = \Lambda(\hat{A}_{11}, \hat{B}_{11}) = \Xi^2 \end{cases},$$

and we assume that Ξ^1 and Ξ^2 are disjoint sets.

Swapping 2×2 blocks: characterization

Lemma: Kågström (1993)

Let the pencil (A, B) be as in (1). Let $X, Y \in \mathbb{R}^{n_1 \times n_2}$ be the solution of:

$$\begin{cases} A_{11}Y - XA_{22} = A_{12}, \\ B_{11}Y - XB_{22} = B_{12}. \end{cases} \tag{2}$$

Then a pair of right deflating subspaces for (A_{22}, B_{22}) are spanned by the columns of:

$$\begin{bmatrix} -Y \\ I_{n_2} \end{bmatrix}, \quad \begin{bmatrix} -X \\ I_{n_2} \end{bmatrix}. \tag{3}$$

Similarly, a pair of left deflating subspaces for (A_{11}, B_{11}) is given by the row spaces of:

$$\begin{bmatrix} I_{n_1} & X \end{bmatrix}, \quad \begin{bmatrix} I_{n_1} & Y \end{bmatrix}. \tag{4}$$

Swapping 2×2 blocks: characterization (cont.)

Moreover, the orthogonal equivalence transformations Q and Z swap the spectra of the diagonal blocks in $Q^T(A, B)Z$ if and only if:

$$\begin{bmatrix} -Y \\ I_{n_2} \end{bmatrix} = Z \begin{bmatrix} R_Y \\ 0 \end{bmatrix}, \quad \text{and} \quad \begin{bmatrix} I_{n_1} & X \end{bmatrix} = \begin{bmatrix} 0 & R_X \end{bmatrix} Q^T, \tag{5}$$

where R_X and R_Y are square and invertible.

Swapping 2×2 blocks: accuracy

Lemma: Kågström (1993)

Let $\tilde{X}$ and $\tilde{Y}$ be the computed solutions of the generalized Sylvester equation (2). Let

$$E = -A_{12} - A_{11}\tilde{Y} + \tilde{X}A_{22}, \quad \text{and,} \quad F := -B_{12} - B_{11}\tilde{Y} + \tilde{X}B_{22},$$

be their residuals and let $\tilde{Q}$ and $\tilde{Z}$ be the computed factors of the QR factorizations

$$\begin{bmatrix} -\tilde{Y} \\ I \end{bmatrix} = \tilde{Z}\begin{bmatrix} \tilde{R}_Y \\ 0 \end{bmatrix}, \quad \begin{bmatrix} I \\ \tilde{X}^T \end{bmatrix} = \tilde{Q}\begin{bmatrix} 0 \\ \tilde{R}_X^T \end{bmatrix}.$$

Then the computed equivalence transformation satisfies:

$$\left(\begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} \\ \Delta_A & \tilde{A}_{22} \end{bmatrix}, \begin{bmatrix} \tilde{B}_{11} & \tilde{B}_{12} \\ \Delta_B & \tilde{B}_{22} \end{bmatrix} \right) = \tilde{Q}^T \left(\begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}, \begin{bmatrix} B_{11} & B_{12} \\ 0 & B_{22} \end{bmatrix} \right) \tilde{Z},$$

Swapping 2×2 blocks: accuracy (cont.)

where,

$$\|\Delta_A\|_2 \leq \|E\|_F / \sqrt{(1 + \sigma_2(X)^2)(1 + \sigma_2(Y)^2)},$$
$$\|\Delta_B\|_2 \leq \|F\|_F / \sqrt{(1 + \sigma_2(X)^2)(1 + \sigma_2(Y)^2)}.$$

This does *not* imply that $\mathrm{t}(\Delta_A, \Delta_B)$ can be safely dismissed according to $\|\Delta_A\| \leq \epsilon_m \|A\|_2$, $\|\Delta_B\| \leq \epsilon_m \|B\|_2$. Nevertheless, the bound is often pessimistic.

Swapping 2×2 blocks: refinement (C.-Mastronardi-Vandebril-Van Dooren, 2019)

$$\left(\begin{bmatrix} A_{11} & A_{12} \\ \Delta_A & A_{22} \end{bmatrix}, \begin{bmatrix} B_{11} & B_{12} \\ \Delta_B & B_{22} \end{bmatrix} \right) \tag{6}$$

System of quadratic matrix equations:

$$\begin{aligned} \Delta_A - A_{22}Y + XA_{11} - XA_{12}Y &= 0, \\ \Delta_B - B_{22}Y + XB_{11} - XB_{12}Y &= 0, \end{aligned}$$

for $X, Y \in \mathbb{R}^{n_1 \times n_2}$. Approximated by the system of linear matrix equations:

$$\begin{aligned} \Delta_A &= A_{22}Y - XA_{11}, \\ \Delta_B &= B_{22}Y - XB_{11}, \end{aligned}$$

Swapping 2×2 blocks: refinement (C.-Mastronardi-Vandebril-Van Dooren, 2019) (cont.)

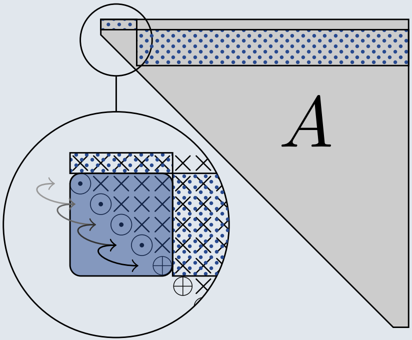
Orthonormal equivalence transformation:

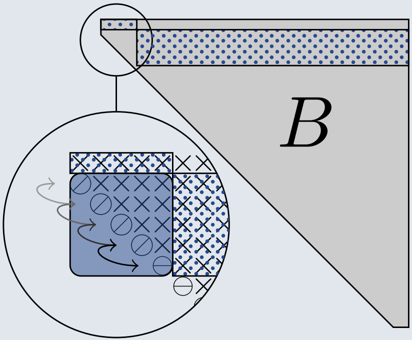
$$Q_{up} = \begin{bmatrix} I_{n_2} & X^T \\ -X & I_{n_1} \end{bmatrix} \begin{bmatrix} R_X & 0 \\ 0 & R_{X^T} \end{bmatrix}, \quad Z_{up} = \begin{bmatrix} I_{n_2} & Y^T \\ -Y & I_{n_1} \end{bmatrix} \begin{bmatrix} R_Y & 0 \\ 0 & R_{Y^T} \end{bmatrix}$$

where R_X, R_{X^T} R_Y and R_{Y^T} normalize Q_{up} and Z_{up} as orthonormal.

Multishift, multipole rational QZ

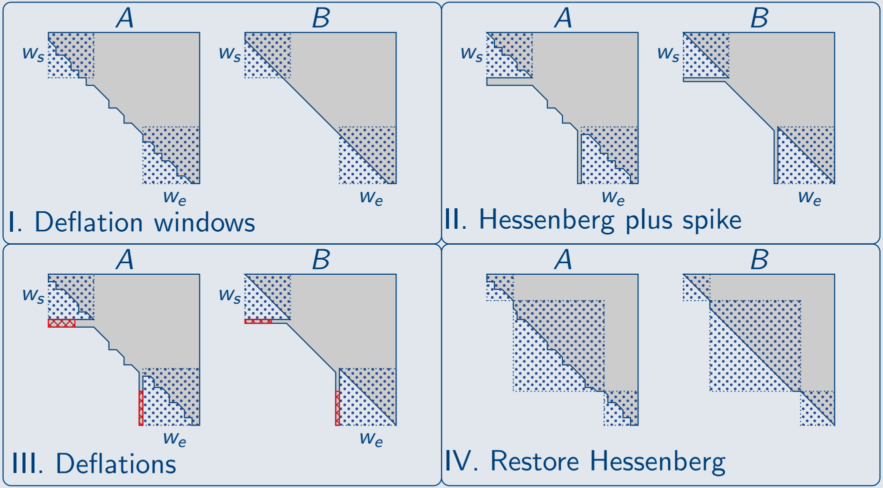
Batched operations





Multishift, multipole rational QZ

Aggressive early deflation (Braman-Byers-Mathias, 2002)



Multishift, multipole rational QZ

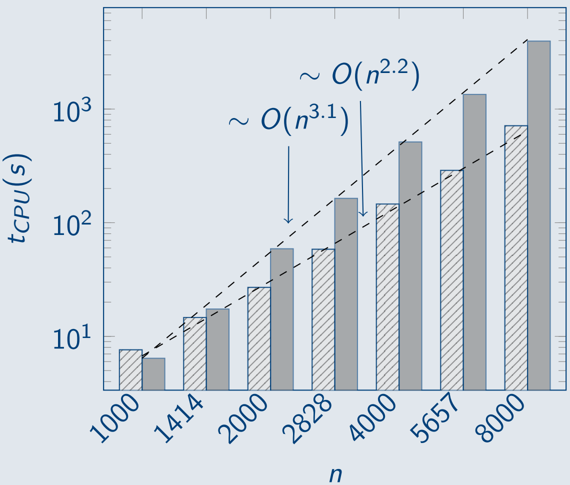
Heuristics

Table 3: `libRQZ` settings: n problem size, m step multiplicity, k swap range, w_e AED window size at the bottom-right side of the pencil, w_s AED window size at the upper-left side of the pencil.

n	m	k	w_e	w_s
$[1; 80[$	1—2	1—2	1—2	1—2
$[80; 150[$	4	4	6	4
$[150; 250[$	8	8	10	4
$[250; 501[$	16	16	18	6
$[501; 1001[$	32	32	34	10
$[1001; 3000[$	64	64	66	16
$[3000; 6000[$	128	128	130	32
$[6000; \infty[$	256	256	266	48

Multishift, multipole rational QZ

Numerical experiments with `libRQZ v0.1`



Rational QR

Pole swapping for $A\boldsymbol{x} = \lambda\boldsymbol{x}$

The solution of $A\boldsymbol{x} = \lambda\boldsymbol{x}$ is often of practical interest.

Pole swapping for $Ax = \lambda x$

Francis' QR method

$$
\begin{matrix}
\times & \times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times & \times \\
 & \times & \times & \times & \times & \times & \times & \times \\
 & & \times & \times & \times & \times & \times & \times \\
 & & & \times & \times & \times & \times & \times \\
 & & & & \times & \times & \times & \times \\
 & & & & & \times & \times & \times \\
 & & & & & & \times & \times
\end{matrix}
$$

$$A$$

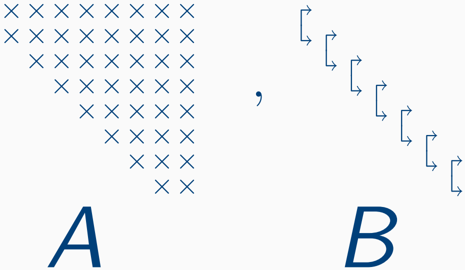
Pole swapping for $Ax = \lambda x$

Our rational QZ method

$$
\underset{A}{\begin{matrix}
\times & \times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times & \times \\
 & \times & \times & \times & \times & \times & \times & \times \\
 & & \times & \times & \times & \times & \times & \times \\
 & & & \times & \times & \times & \times & \times \\
 & & & & \times & \times & \times & \times \\
 & & & & & \times & \times & \times \\
 & & & & & & \times & \times
\end{matrix}}
,\quad
\underset{B}{\begin{matrix}
\times & \times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times & \times \\
 & \times & \times & \times & \times & \times & \times & \times \\
 & & \times & \times & \times & \times & \times & \times \\
 & & & \times & \times & \times & \times & \times \\
 & & & & \times & \times & \times & \times \\
 & & & & & \times & \times & \times \\
 & & & & & & \times & \times
\end{matrix}}
$$

Pole swapping for $Ax = \lambda x$

Our rational QZ method for $Ax = \lambda x$: Rational QR

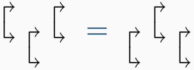


Pole swapping for $Ax = \lambda x$

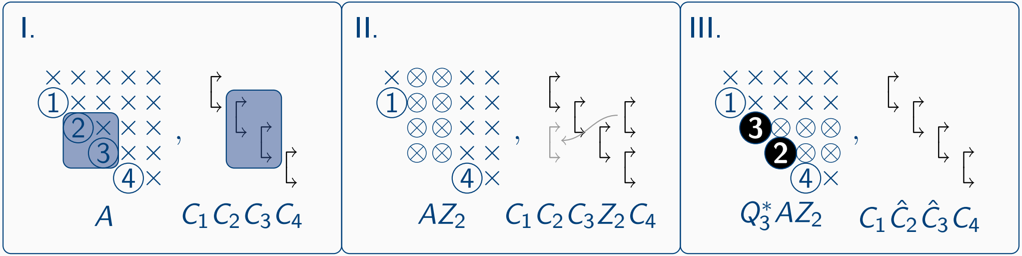
Core transformations:

$$= \begin{bmatrix} c & -s \\ s & \bar{c} \end{bmatrix}$$

Turnover operation:

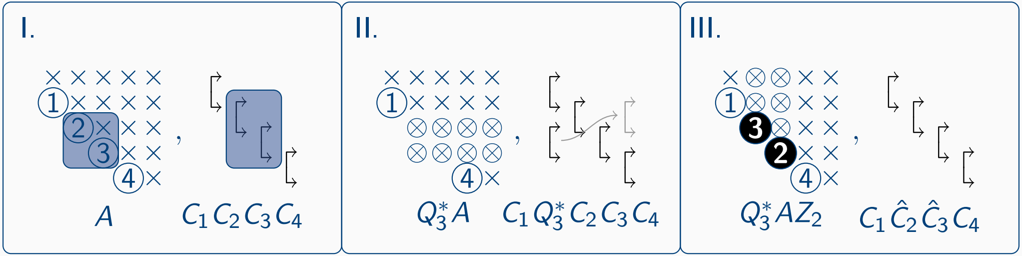


Pole swapping for $Ax = \lambda x$



$$|\xi_2| \geq |\xi_3|$$

Pole swapping for $Ax = \lambda x$



$|\xi_2| < |\xi_3|$

Pole swapping for $Ax = \lambda x$

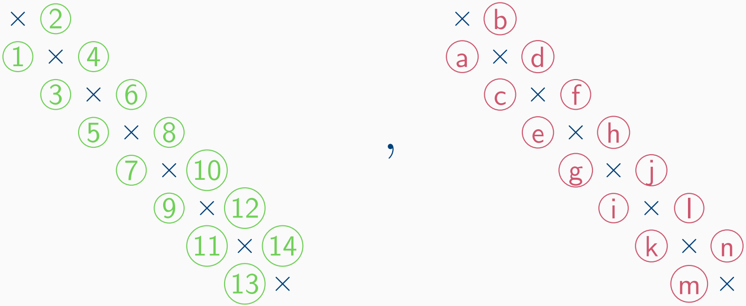
n	# runs	ZLAHQR $t_{CPU}(s)$	ZLAHPS $t_{CPU}(s)$	% t_{CPU}
5	1000	$1.4 \cdot 10^{-5}$	$1.4 \cdot 10^{-5}$	100%
10	1000	$6.0 \cdot 10^{-5}$	$5.6 \cdot 10^{-5}$	93%
20	500	$2.8 \cdot 10^{-4}$	$2.4 \cdot 10^{-4}$	86%
40	250	$1.6 \cdot 10^{-3}$	$1.3 \cdot 10^{-3}$	81%
80	125	$1.0 \cdot 10^{-2}$	$7.4 \cdot 10^{-3}$	74%
150	80	$6.3 \cdot 10^{-2}$	$4.5 \cdot 10^{-2}$	71%
300	80	$5.0 \cdot 10^{-1}$	$3.2 \cdot 10^{-1}$	64%
600	40	$3.6 \cdot 10^{0}$	$2.3 \cdot 10^{0}$	64%
1000	40	$1.6 \cdot 10^{1}$	$1.0 \cdot 10^{1}$	63%

Pole swapping for $Ax = \lambda x$

n	$\#$ runs	`ZLAHQR` BWE	`ZLAHPS` BWE
5	1000	$1.8 \cdot 10^{-15}$	$1.2 \cdot 10^{-15}$
10	1000	$1.8 \cdot 10^{-15}$	$1.4 \cdot 10^{-15}$
20	500	$2.8 \cdot 10^{-15}$	$1.8 \cdot 10^{-15}$
40	250	$3.7 \cdot 10^{-15}$	$2.6 \cdot 10^{-15}$
80	125	$5.7 \cdot 10^{-15}$	$3.7 \cdot 10^{-15}$
150	80	$7.8 \cdot 10^{-15}$	$4.9 \cdot 10^{-15}$
300	80	$1.1 \cdot 10^{-14}$	$6.9 \cdot 10^{-15}$
600	40	$1.5 \cdot 10^{-14}$	$9.5 \cdot 10^{-15}$
1000	40	$2.0 \cdot 10^{-14}$	$1.2 \cdot 10^{-14}$

Rational LR and TTT

Rational LR and TTT



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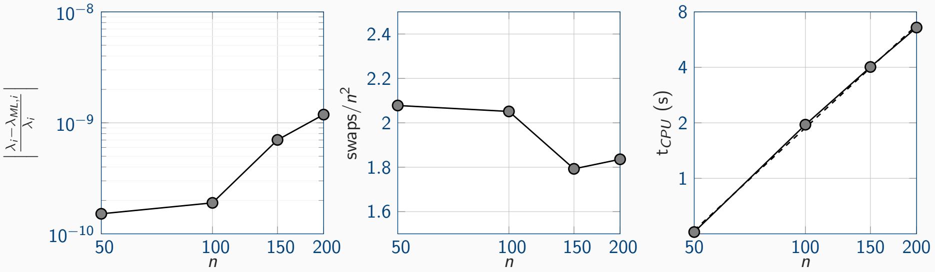
Rational LR and TTT



Conclusion

Conclusion and outlook

1. We have presented a novel interpretation of QR-type methods:

   $$\textit{bulge chasing} \leftrightarrow \textit{pole swapping}.$$

2. This results in a more general class of algorithms
3. Convergence is determined by rational functions instead of polynomials
4. Faster and more flexible eigensolvers
5. Premature deflations during reduction
6. Backward stable
7. Explored the use of blocking and advanced deflation techniques (speedup with factor 6)
8. Applied the same principle to standard eigenvalue problem (speedup of 30%)
9. Tridiagonal generalized eigenvalue problems in $O(n^2)$ complexity

References

Arnoldi, W. E. (1951). The principle of minimized iteration in the solution of the matrix eigenvalue problem. *Quart. Appl. Math.*, 9:17–29.

Berljafa, M., and Güttel, S. (2015). Generalized rational Krylov decompositions with an application to rational approximation. *SIMAX*, 36(2):894–916.

Braman, K., Byers R., and Mathias, R. (2002) The multishift QR algorithm. Part II: aggressive early deflation. *SIMAX*, 23(4):948–973.

Camps, D., Meerbergen, K., and Vandebril, R. (2019). A rational QZ method. *SIMAX* 40(30):943–972.

Camps, D., Meerbergen, K., and Vandebril, R. (2019). A multishift, multipole rational QZ method with aggressive early deflation. Submitted.

Camps, D., Mach, T., Vandebril, R., and Watkins, D. S. (2019). On pole-swapping algorithms for the eigenvalue problem. Submitted.

Camps, D. (2019). Pole swapping methods for the eigenvalue problem – rational QR algorithms. PhD thesis.

Camps, D., Mastronardi, N., Vandebril, R., and Van Dooren P. (2019). Swapping 2×2 blocks in the Schur and generalized Schur form. *JCAM* Available online.

References (cont.)

Elsner, L., and Watkins, D. S. Convergence of algorithms of decomposition type for the eigenvalue problem. *Lin. Alg. Appl.*, 143:19–47.

Francis, J. G. F. (1961-62) The QR transformation, a unitary analogue to the LR transformation — Part 1 and 2 *The Computer Journal*.

Kågström, B. (1993) A direct method for reordering eigenvalues in the generalized real Schur form of a regular matrix pair (A, B). In *Linear Algebra for Large Scale and Real-Time Applications*.

Kublanovskaya, V. N. (1961) On some algorithms for the solution of the complete eigenvalue problem *USSR Comp. Math. Phys.* In Russian.

Moler, C. B., and Stewart, G. W. (1973) An algorithm for generalized matrix eigenvalue problems. *SIAM J. Numer. Anal.*, 10(2):241–256.

Ruhe, A. (1998) Rational Krylov: A practical algorithm for large sparse nonsymmetric matrix pencils. *SISC*, 19(5):1535–1551

Van Dooren, P. (1981) A generalized eigenvalue approach for solving Riccati equations *SISC*, 2(2):121–135

Watkins, D. S. (1993) Some perspectives on the eigenvalue problem. *SIREV*, 35:430–471.