A rational QZ method

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

Overview

We will discuss:

Numerical solution of the generalized eigenvalue problem:

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- ♢ Small to medium-sized
- ♢ Regular
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- Shift & *pole* introduction and swapping
- Rational Krylov
- Nested subspace iteration

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  $\rightarrow$ generalization of the classic QZ method `[Moler and Stewart]`

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Generalized eigenvalue problems

- Given A & B: $n \times n$ matrices, either $\mathbb{R}$ or $\mathbb{C}$
- Computation of the triplets $(\alpha, \beta, \boldsymbol{x})$ that satisfy $\beta A\boldsymbol{x} = \alpha B\boldsymbol{x}$
- Procedure:
  1. Reduce the pencil to *manageable* form
  2. Iterate to generalized Schur form
  3. Recover eigenvectors
- Make use of well-chosen unitary equivalences:

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

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Tools

Hessenberg, Hessenberg form

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

Tools

Hessenberg, Hessenberg form

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

$$A \qquad\qquad B$$

Tools

Hessenberg, Hessenberg form

$$
\begin{array}{cccccccc}
\times & \times & \times & \times & \times & \times & \times & \times \\
{\color{green}\times} & \times & \times & \times & \times & \times & \times & \times \\
 & {\color{green}\times} & \times & \times & \times & \times & \times & \times \\
 & & {\color{green}\times} & \times & \times & \times & \times & \times \\
 & & & {\color{green}\times} & \times & \times & \times & \times \\
 & & & & {\color{green}\times} & \times & \times & \times \\
 & & & & & {\color{green}\times} & \times & \times \\
 & & & & & & {\color{green}\times} & \times
\end{array}
\quad , \quad
\begin{array}{cccccccc}
\times & \times & \times & \times & \times & \times & \times & \times \\
{\color{red}\times} & \times & \times & \times & \times & \times & \times & \times \\
 & {\color{red}\times} & \times & \times & \times & \times & \times & \times \\
 & & {\color{red}\times} & \times & \times & \times & \times & \times \\
 & & & {\color{red}\times} & \times & \times & \times & \times \\
 & & & & {\color{red}\times} & \times & \times & \times \\
 & & & & & {\color{red}\times} & \times & \times \\
 & & & & & & {\color{red}\times} & \times
\end{array}
$$

$$A \qquad\qquad B$$

$$\text{poles } \Xi = \left(\frac{{\color{green}\times}}{{\color{red}\times}}, \frac{{\color{green}\times}}{{\color{red}\times}}, \ldots\right)$$

Tools

Hessenberg, Hessenberg form

$$
\underbrace{\begin{matrix}
\times & \times & \times & \times & \times & \times & \times & \times \\
\textcircled{1} & \times & \times & \times & \times & \times & \times & \times \\
 & \textcircled{2} & \times & \times & \times & \times & \times & \times \\
 & & \textcircled{3} & \times & \times & \times & \times & \times \\
 & & & \textcircled{4} & \times & \times & \times & \times \\
 & & & & \textcircled{5} & \times & \times & \times \\
 & & & & & \textcircled{6} & \times & \times \\
 & & & & & & \textcircled{7} & \times
\end{matrix}}_{A}
\quad , \quad
\underbrace{\begin{matrix}
\times & \times & \times & \times & \times & \times & \times & \times \\
\textcircled{a} & \times & \times & \times & \times & \times & \times & \times \\
 & \textcircled{b} & \times & \times & \times & \times & \times & \times \\
 & & \textcircled{c} & \times & \times & \times & \times & \times \\
 & & & \textcircled{d} & \times & \times & \times & \times \\
 & & & & \textcircled{e} & \times & \times & \times \\
 & & & & & \textcircled{f} & \times & \times \\
 & & & & & & \textcircled{g} & \times
\end{matrix}}_{B}
$$

$$\text{poles } \Xi = \left(\frac{\textcircled{1}}{\textcircled{a}}, \frac{\textcircled{2}}{\textcircled{b}}, \ldots\right)$$

Tools

Hessenberg, triangular form (QZ)

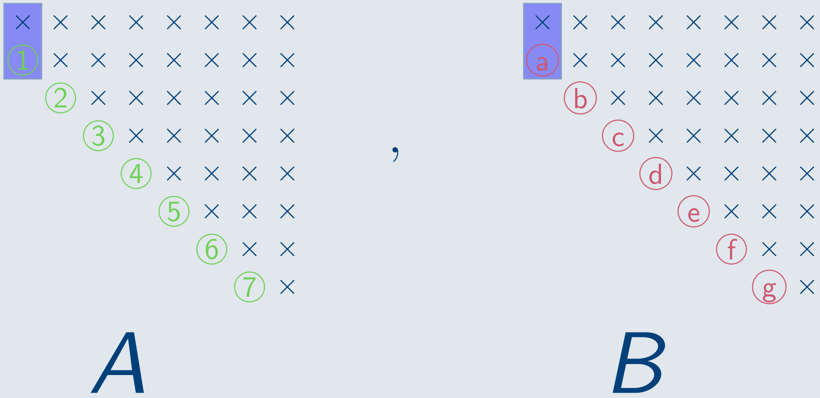
$$
\begin{matrix}
\times & \times & \times & \times & \times & \times & \times & \times \\
① & \times & \times & \times & \times & \times & \times & \times \\
 & ② & \times & \times & \times & \times & \times & \times \\
 & & ③ & \times & \times & \times & \times & \times \\
 & & & ④ & \times & \times & \times & \times \\
 & & & & ⑤ & \times & \times & \times \\
 & & & & & ⑥ & \times & \times \\
 & & & & & & ⑦ & \times
\end{matrix}
\quad , \quad
\begin{matrix}
\times & \times & \times & \times & \times & \times & \times & \times \\
\mathbf{0} & \times & \times & \times & \times & \times & \times & \times \\
 & \mathbf{0} & \times & \times & \times & \times & \times & \times \\
 & & \mathbf{0} & \times & \times & \times & \times & \times \\
 & & & \mathbf{0} & \times & \times & \times & \times \\
 & & & & \mathbf{0} & \times & \times & \times \\
 & & & & & \mathbf{0} & \times & \times \\
 & & & & & & \mathbf{0} & \times
\end{matrix}
$$

$$A \qquad\qquad B$$

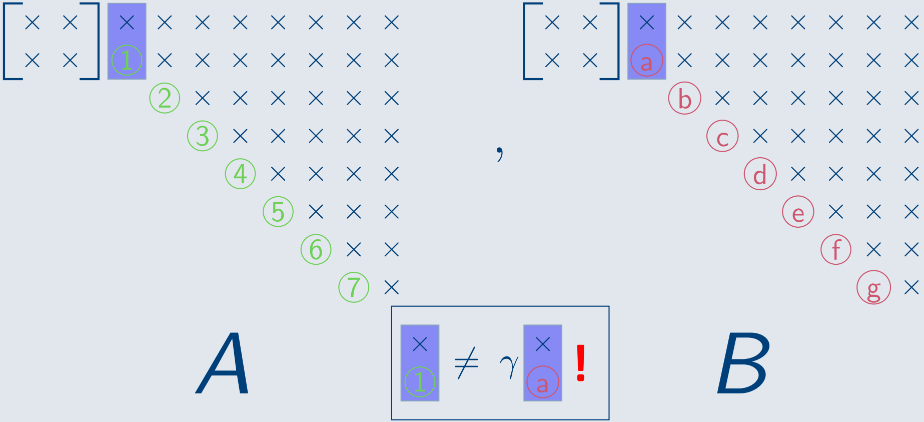
$$\text{poles } \Xi = \left(\frac{①}{0}, \frac{②}{0}, \ldots\right)$$

Tools: manipulating the Hessenberg pencil

Changing the first pole/Introducing a shift



Changing the first pole/Introducing a shift



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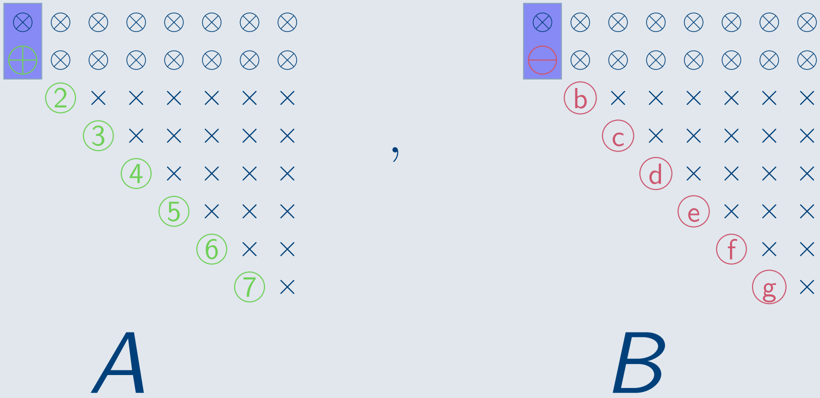

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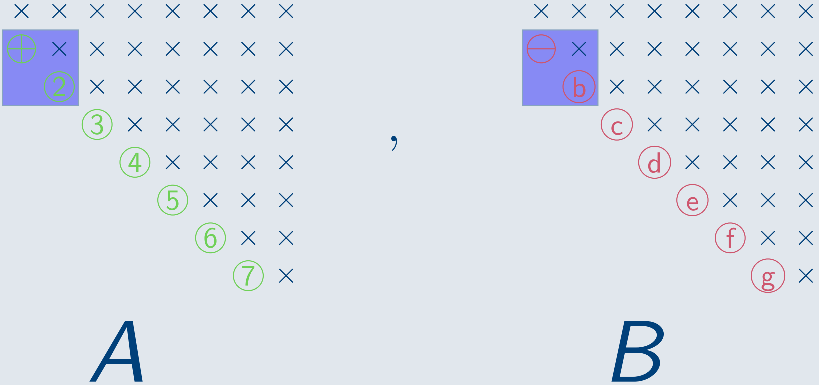
Swapping consecutive poles



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Swapping consecutive poles

This problem is completely analogous to reordering eigenvalues in the Schur form.

- [Kågström and Poromaa]: solution of a coupled Sylvester equation $(k \times k)$
- [Bojanczyk and Van Dooren]: direct method $(1 \times 1$ or $2 \times 2)$

<u>Conditions:</u>

$$\frac{\oplus}{\ominus} \neq \frac{\textcircled{2}}{\textcircled{b}} \; ! \qquad \frac{\oplus}{\ominus} \neq \frac{0}{0} \; ! \qquad \frac{\textcircled{2}}{\textcircled{b}} \neq \frac{0}{0} \; !$$

$$\Rightarrow Q^* = \begin{bmatrix} \times & \times \\ \times & \times \end{bmatrix}, Z = \begin{bmatrix} \times & \times \\ \times & \times \end{bmatrix}$$

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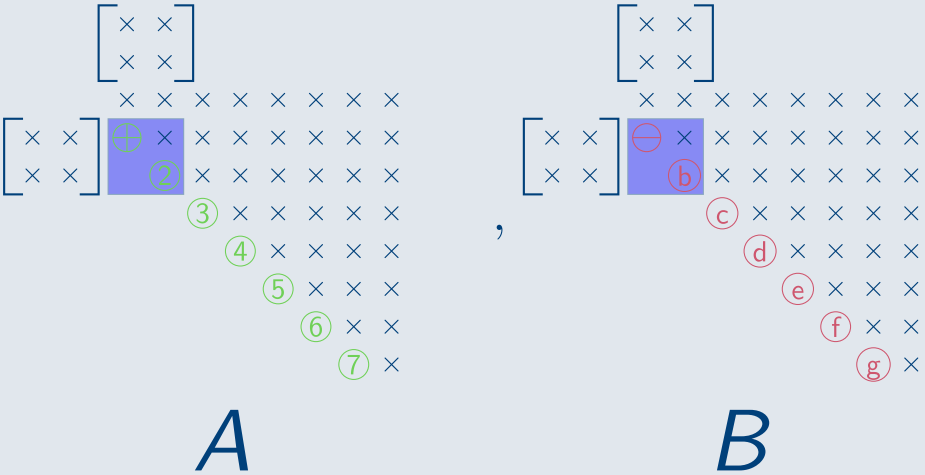
Swapping consecutive poles



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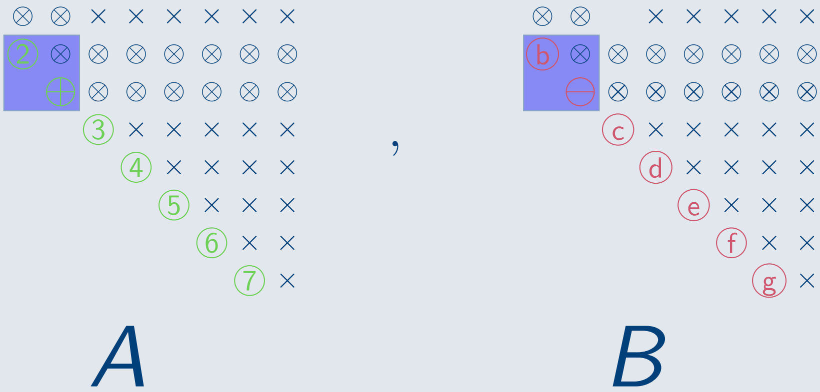

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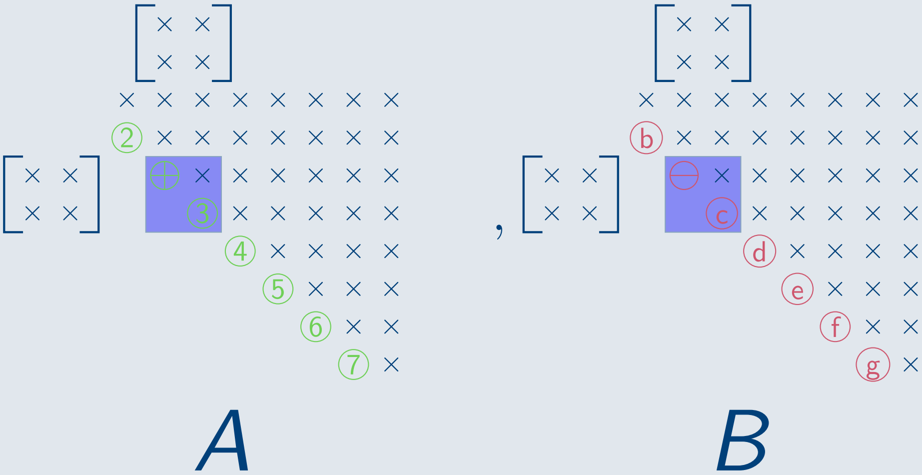

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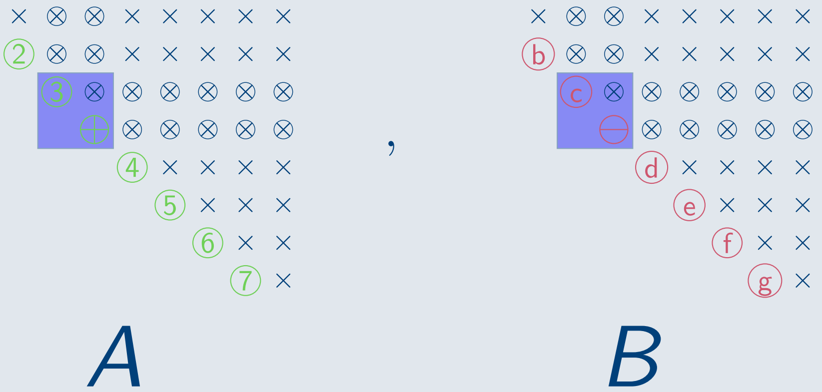

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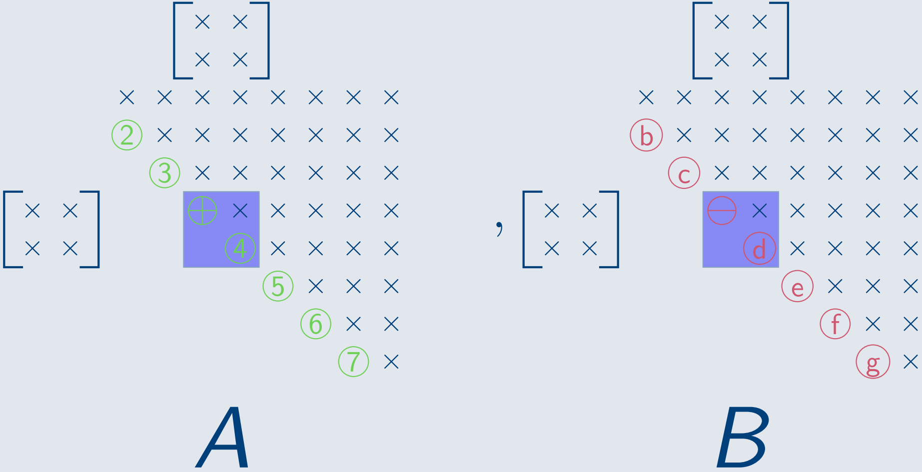

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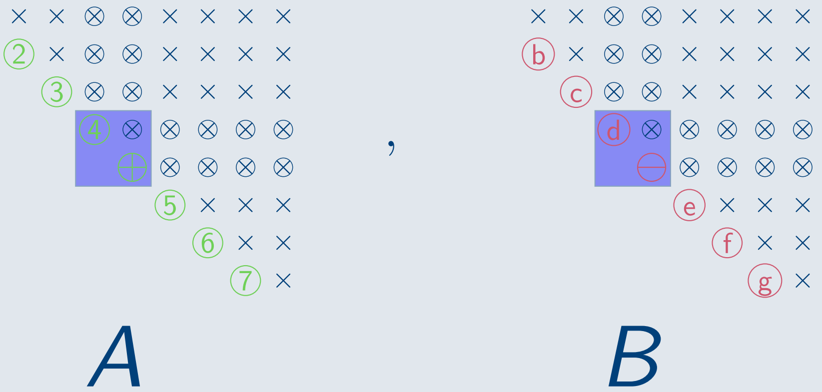

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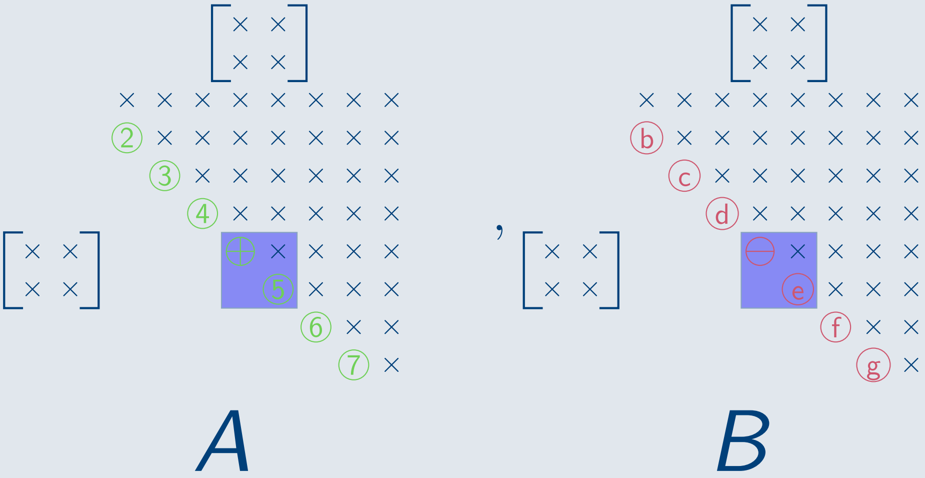

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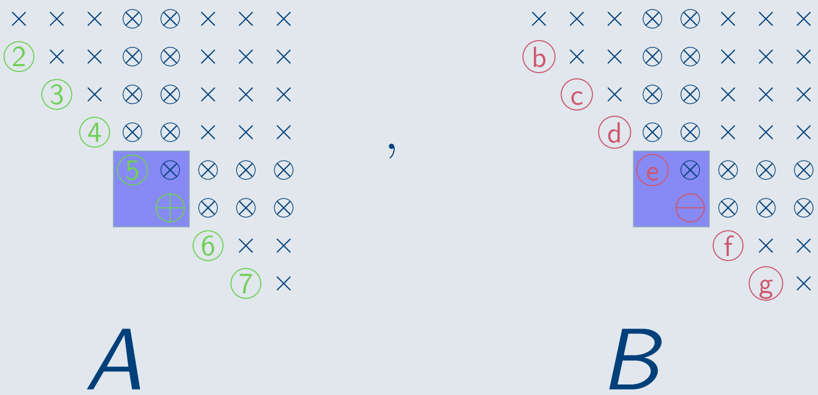

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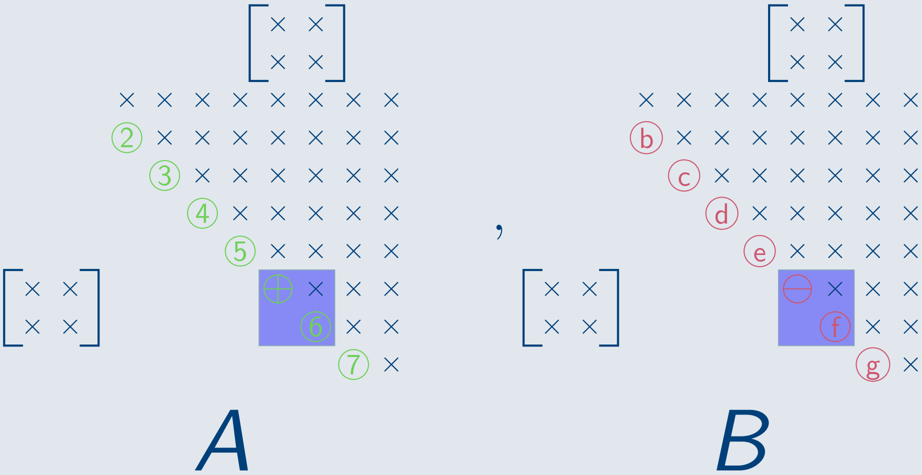

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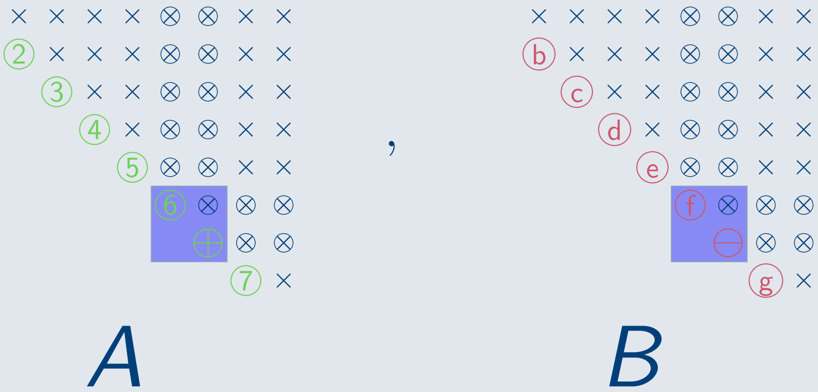

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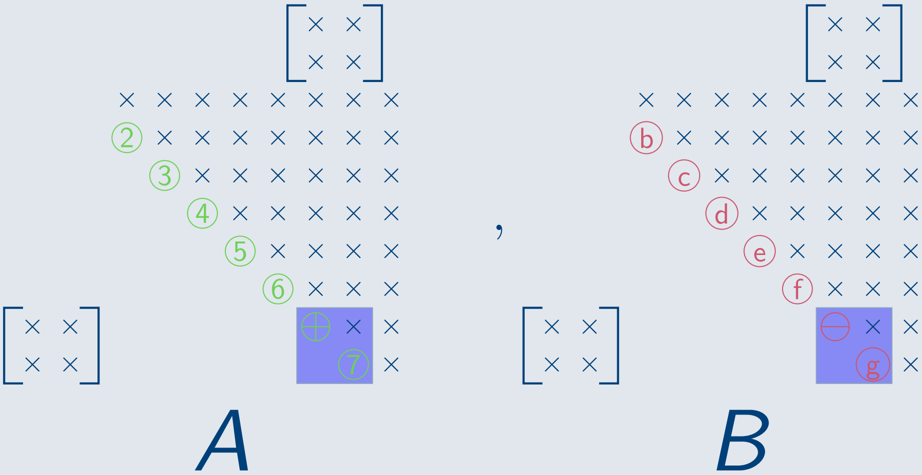

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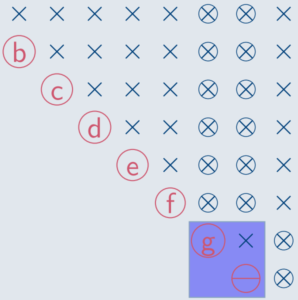
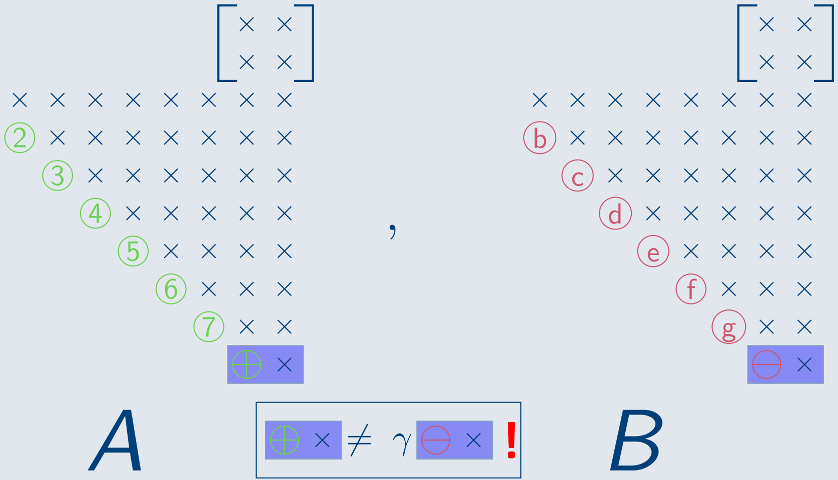
A ,



B

Tools: manipulating the Hessenberg pencil

Changing the last pole/Removing the shift



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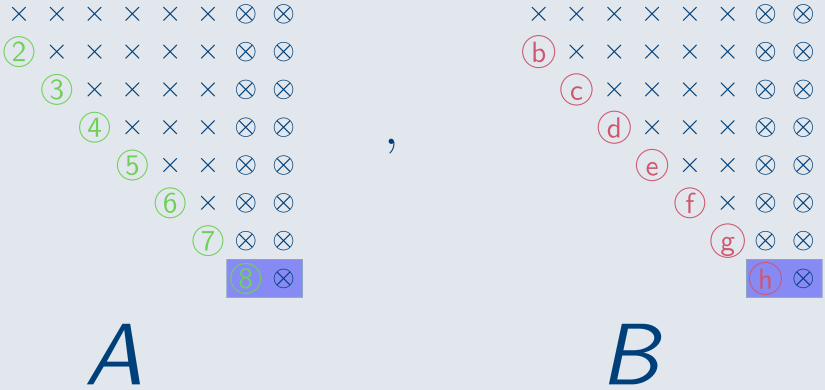

The algorithm in a nutshell:

RQZ algorithm

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1. Introduce shift at the top

RQZ algorithm

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1. Introduce shift at the top
2. Swap it all the way down

RQZ algorithm

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RQZ algorithm

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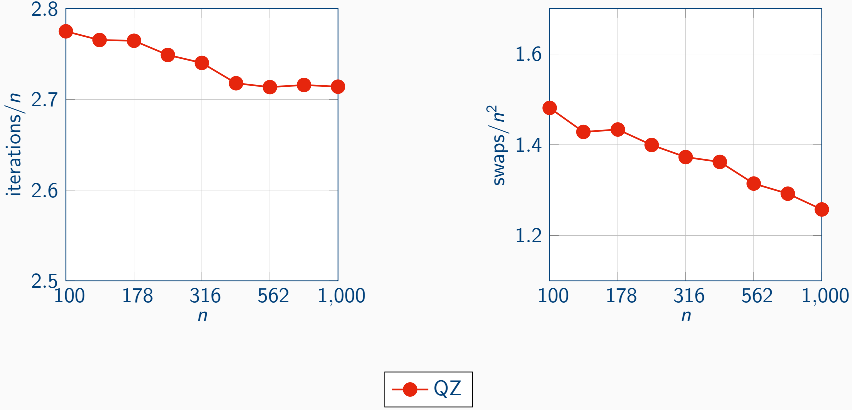
Poles at ∞ **(**$\times = 0$**)** $\rightarrow$ **QZ method**: Bulge exchange interpretation [Watkins]

Caution: shift $\notin \Xi$ to avoid slower convergence

Is it worth it?

Data: 9 random matrix pairs, $n \in [100, 1000]$, reduced to H-T, averaged over 10 runs



Numerical example

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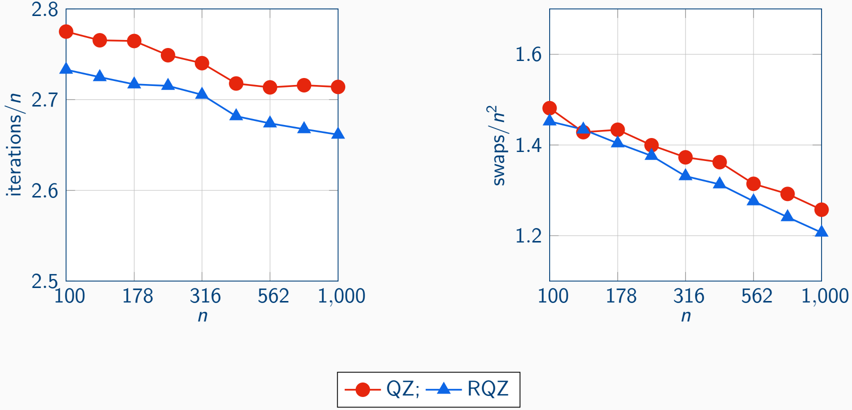

$\Rightarrow$ up to $5 - 10\%$ reduction in iterations with obvious choice of poles.

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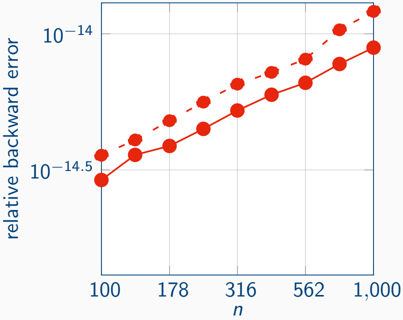

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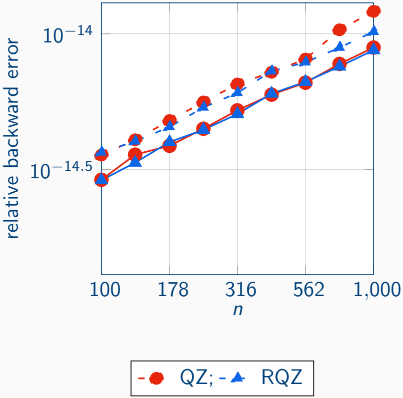


Reduction to Hessenberg form with poles Ξ

Step 1: QR factorization of B

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

$$A \leftarrow Q^* A \qquad B \leftarrow Q^* B$$

Reduction to Hessenberg form with poles Ξ

Step 2: Zero out element $(5,1)$ of A

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

$$A \leftarrow Q_4^* A \qquad B \leftarrow Q_4^* B$$

Reduction to Hessenberg form with poles Ξ

Step 3: Restore upper triangularity of B

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

$$A \leftarrow AZ_4 \qquad B \leftarrow BZ_4$$

Reduction to Hessenberg form with poles Ξ

...Repeat this process on the first column of A until...

Reduction to Hessenberg form with poles Ξ

Step 7: First column of (A, B) in H-T form

$$
\begin{array}{ccccc}
\times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times \\
 & \times & \times & \times & \times \\
 & \times & \times & \times & \times \\
 & \times & \times & \times & \times
\end{array}
\qquad
\begin{array}{ccccc}
\times & \times & \times & \times & \times \\
 & \times & \times & \times & \times \\
 & & \times & \times & \times \\
 & & & \times & \times \\
 & & & & \times
\end{array}
$$

$$A \qquad\qquad\qquad B$$

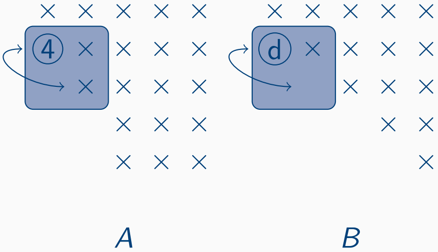
Reduction to Hessenberg form with poles Ξ

Step 7: Change first pole to ξ_{n-1}

$$
\begin{array}{ccccc}
\otimes & \otimes & \otimes & \otimes & \otimes \\
\textcircled{4} & \otimes & \otimes & \otimes & \otimes \\
 & \times & \times & \times & \times \\
 & \times & \times & \times & \times \\
 & \times & \times & \times & \times
\end{array}
\qquad
\begin{array}{ccccc}
\otimes & \otimes & \otimes & \otimes & \otimes \\
\textcircled{d} & \otimes & \otimes & \otimes & \otimes \\
 & & \times & \times & \times \\
 & & & \times & \times \\
 & & & & \times
\end{array}
$$

$A \leftarrow Q_1^* A$ $\qquad$ $B \leftarrow Q_1^* B$

Step 8: Reduce second column to H-T and swap pole 1 and 2



Reduction to Hessenberg form with poles Ξ

Step 9: First pole now at ∞

$$
\begin{array}{ccccc}
\otimes & \otimes & \times & \times & \times \\
\otimes & \otimes & \otimes & \otimes & \otimes \\
 & \textcircled{4} & \otimes & \otimes & \otimes \\
 & & \times & \times & \times \\
 & & \times & \times & \times
\end{array}
\qquad
\begin{array}{ccccc}
\otimes & \otimes & \times & \times & \times \\
 & \otimes & \otimes & \otimes & \otimes \\
 & \textcircled{d} & \otimes & \otimes & \otimes \\
 & & & \times & \times \\
 & & & & \times
\end{array}
$$

$$A \leftarrow Q^* A Z \qquad B \leftarrow Q^* B Z$$

Reduction to Hessenberg form with poles Ξ

Step 10: Change first pole to ξ_{n-2}

$$\begin{matrix} \otimes & \otimes & \otimes & \otimes & \otimes \\ \textcircled{3} & \otimes & \otimes & \otimes & \otimes \\ & \textcircled{4} & \times & \times & \times \\ & & \times & \times & \times \\ & & \times & \times & \times \end{matrix} \qquad \begin{matrix} \otimes & \otimes & \otimes & \otimes & \otimes \\ \textcircled{c} & \otimes & \otimes & \otimes & \otimes \\ & \textcircled{d} & \times & \times & \times \\ & & & \times & \times \\ & & & & \times \end{matrix}$$

$$A \leftarrow Q_1^* A \qquad B \leftarrow Q_1^* B$$

Reduction to Hessenberg form with poles Ξ

... Continue with this process until...

Reduction to Hessenberg form with poles Ξ

End result

$$
\begin{array}{ccccc}
\times & \times & \times & \times & \times \\
\textcircled{1} & \times & \times & \times & \times \\
 & \textcircled{2} & \times & \times & \times \\
 & & \textcircled{3} & \times & \times \\
 & & & \textcircled{4} & \times
\end{array}
\qquad
\begin{array}{ccccc}
\times & \times & \times & \times & \times \\
\textcircled{a} & \times & \times & \times & \times \\
 & \textcircled{b} & \times & \times & \times \\
 & & \textcircled{c} & \times & \times \\
 & & & \textcircled{d} & \times
\end{array}
$$

A B

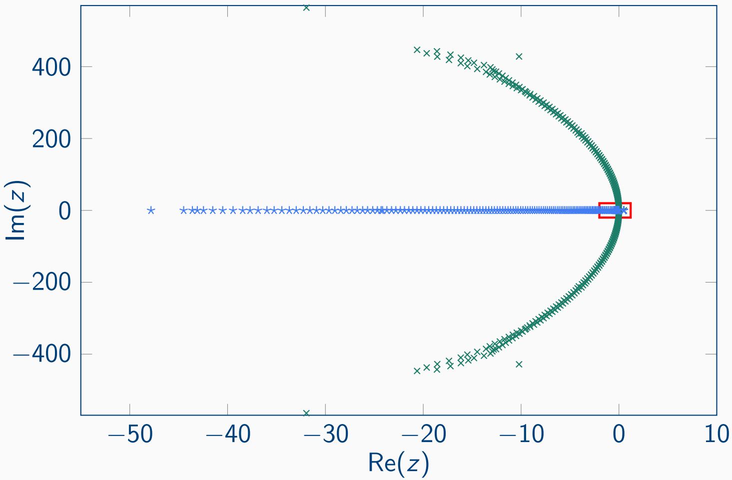
Reduction to Hessenberg form with poles Ξ

Computational cost:

- H-T reduction: $O(8n^3)$ flops
- H-H reduction: additional $O(6n^3)$ flops (worst case)

Numerical example: Reduction to Hessenberg form

Data: MHD matrix pair from MatrixMarket, $n = 1280$



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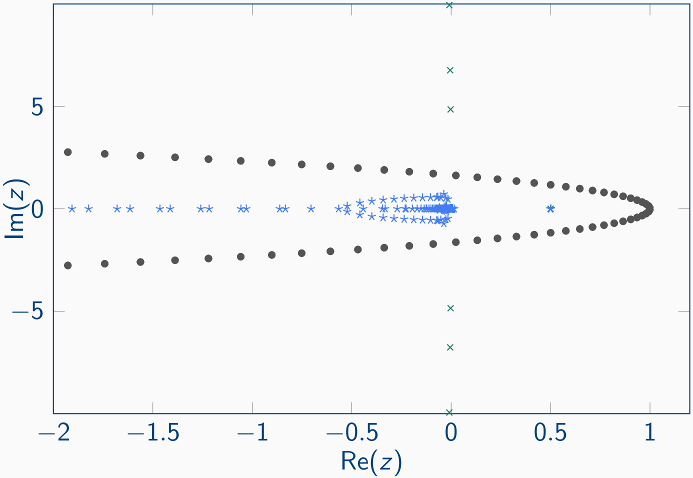

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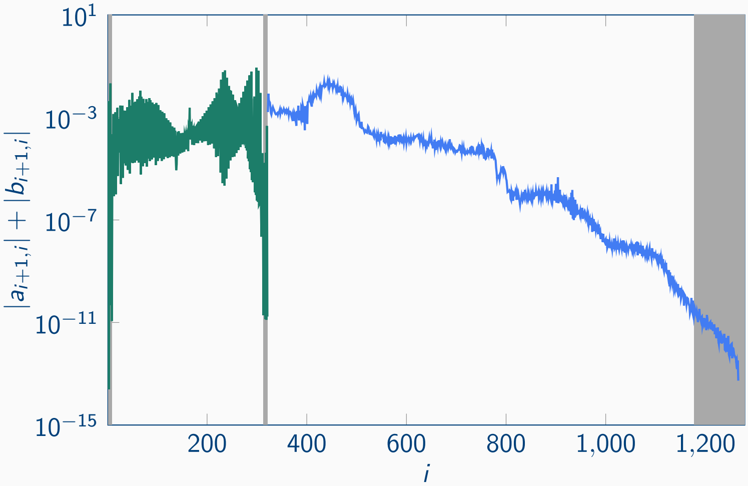
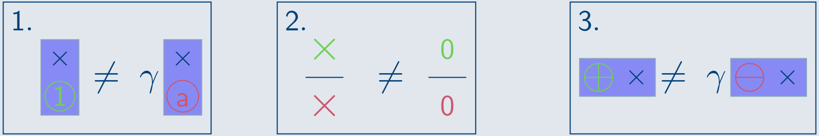


Definition: Properness

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



A word on the theory

Why and how does RQZ work?

Krylov subspaces

1. Krylov subspace: $\mathcal{K}_i(M, \boldsymbol{v}) = \mathcal{R}(\boldsymbol{v}, M\boldsymbol{v}, \ldots, M^{i-1}\boldsymbol{v})$

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2. rational Krylov subspace: $\mathcal{K}_i^{\text{rat}}(M, \boldsymbol{v}, \Xi = (\xi_1, \ldots, \xi_{i-1})) = q_\Xi(M)^{-1}\, \mathcal{K}_i(M, \boldsymbol{v})$

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Theorem

If (A, B) is a proper Hessenberg pair with poles $(\xi_1, \ldots, \xi_{n-1})$ then for $i = 1, \ldots, n{-}1$:

$$\mathcal{K}_i^{\text{rat}}(AB^{-1}, \boldsymbol{e}_1, (\xi_1, \ldots, \xi_{i-1})) = \mathcal{K}_i^{\text{rat}}(B^{-1}A, \boldsymbol{e}_1, (\xi_2, \ldots, \xi_i)) = \mathcal{R}(\boldsymbol{e}_1, \ldots, \boldsymbol{e}_i) = \mathcal{E}_i$$

A word on the theory

Why and how does RQZ work?

Theorem: Implicit Q (and Z)

Given a 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 poles are fixed.

A word on the theory

Why and how does RQZ work?

Nested subspace iteration

An RQZ step with shift ϱ on a Hessenberg pencil with poles $(\xi_1, \ldots, \xi_{n-1})$ and new pole ξ_n performs nested subspace iteration for $i = 1, \ldots, n-1$ accelerated by

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

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What does this mean?

- QR step with shift ϱ on entire space $\rightarrow$ fast convergence at the bottom

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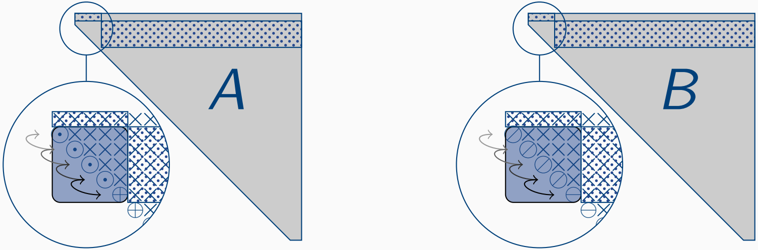
What does this mean?

- QR step with shift ϱ on entire space $\to$ fast convergence at the bottom
- RQ steps with tightly packed shifts Ξ on selected subspaces $\to$ slow convergence at the top

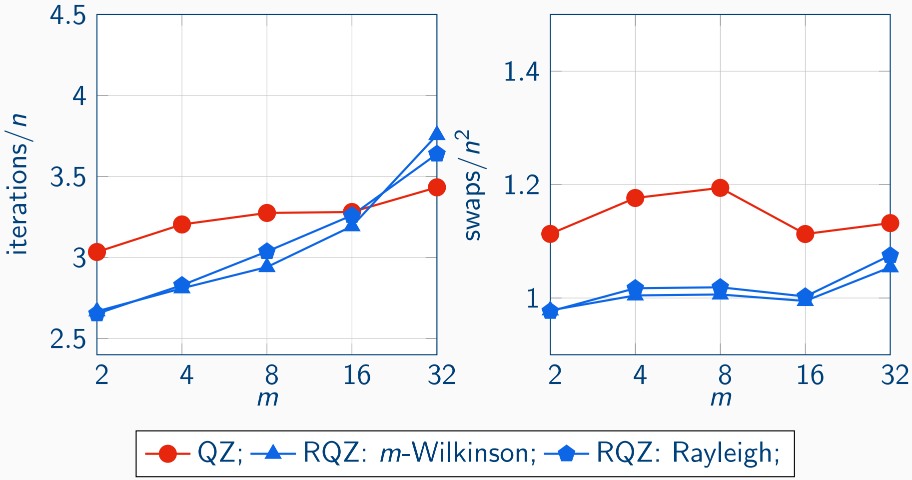
Further extensions

Tightly packed shifts



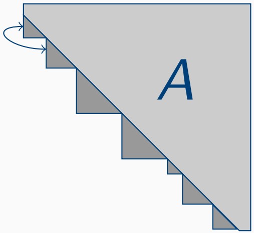
→ More cache efficient implementations (Level 3 BLAS)

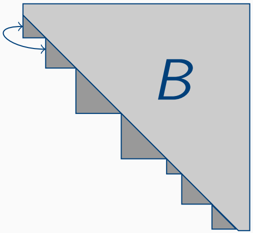
Tightly packed shifts



Further extensions

Block Hessenberg

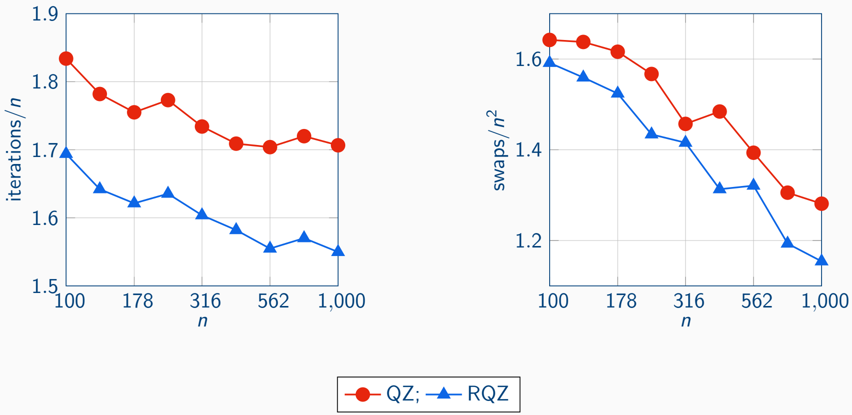




→ complex conjugate shifts and poles in real arithmetic for real pencils

Block Hessenberg

Data: 9 real-valued random matrix pairs, $n \in [100, 1000]$, reduced to H-T, averaged over 5 runs



Conclusions

1. RQZ is a generalization of QZ: *bulge chasing* $\leftrightarrow$ *pole swapping*
2. Implicit rational subspace iteration is promising
3. New shift and pole strategies can be a powerful tool to compute invariant subspaces (already during reduction of the pencil)

Further reading:

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Thank you for your attention!