KU LEUVEN

A rational QZ method

Daan Camps

joint work with: Karl Meerbergen and Raf Vandebril

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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
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- ♢ Shift & *pole* introduction and swapping
- ♢ Rational Krylov
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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
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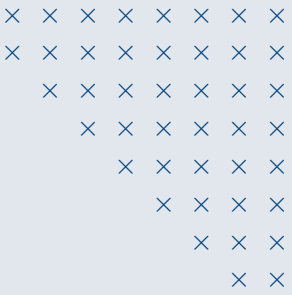

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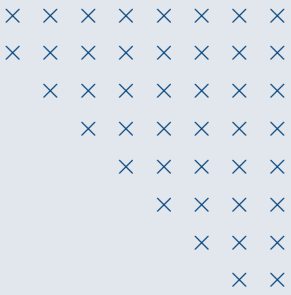

B

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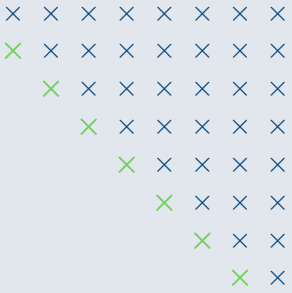

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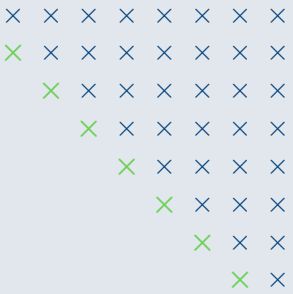

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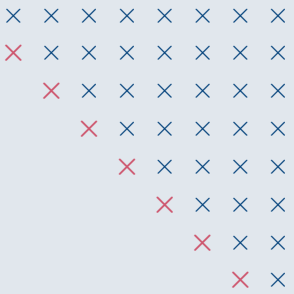

A B

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

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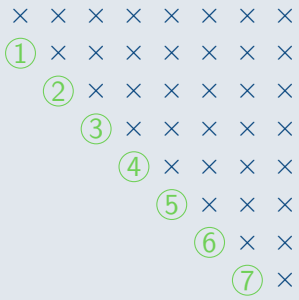

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A B

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

Tools

Hessenberg, triangular form (QZ)

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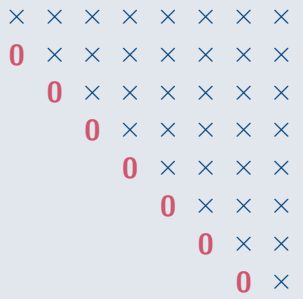

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$$\text{poles } \Xi = \left(\frac{①}{0}, \frac{②}{0}, \ldots\right)$$

Tools: manipulating the Hessenberg pencil

Changing the first pole/Introducing a shift

A

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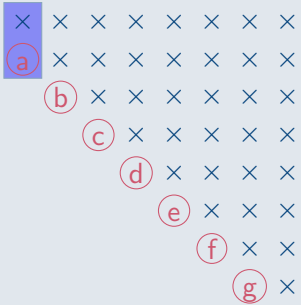

B

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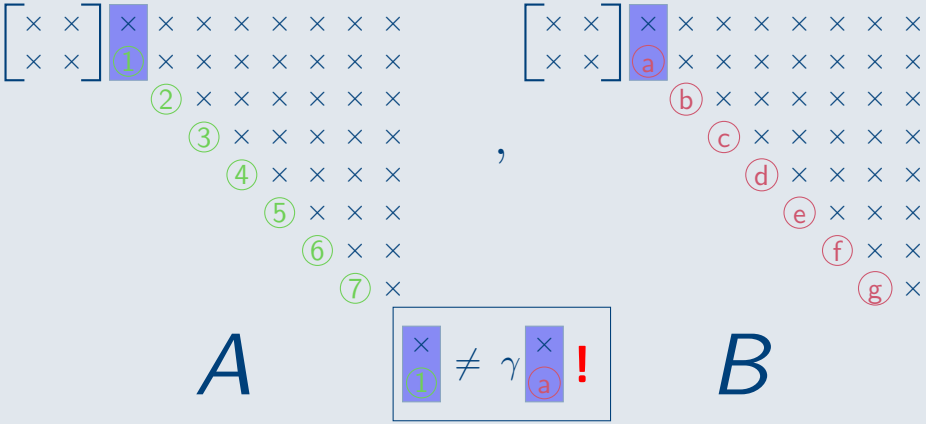

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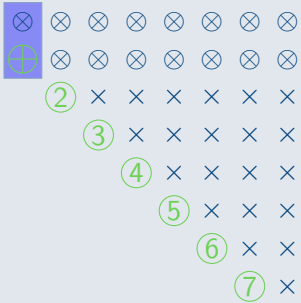

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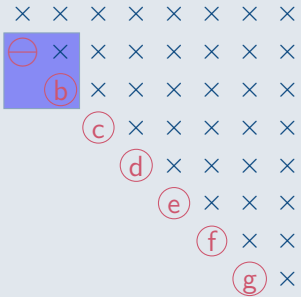

B

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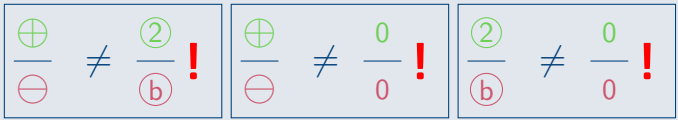
Swapping consecutive poles

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 (1×1 or 2×2)

Conditions:



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

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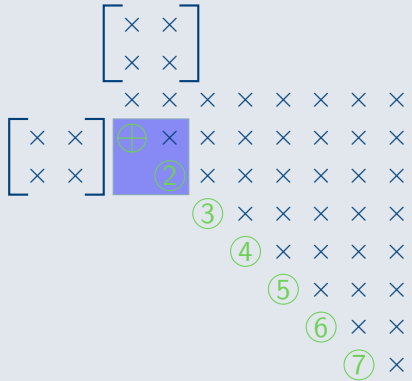

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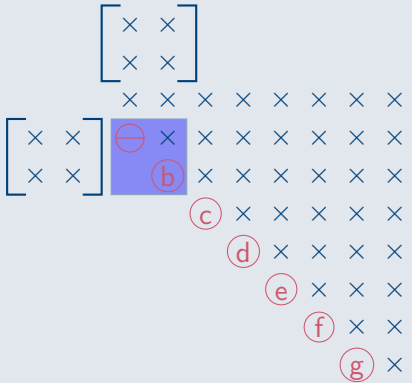

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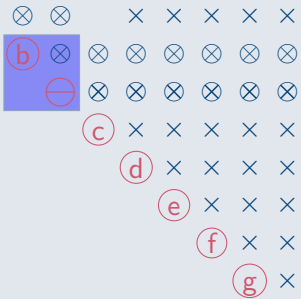

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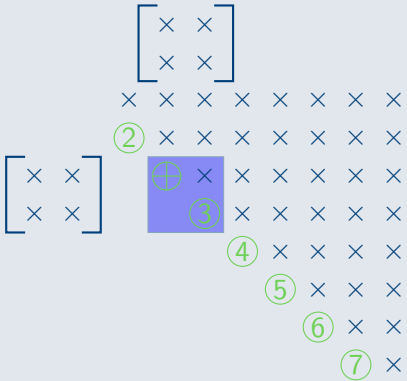

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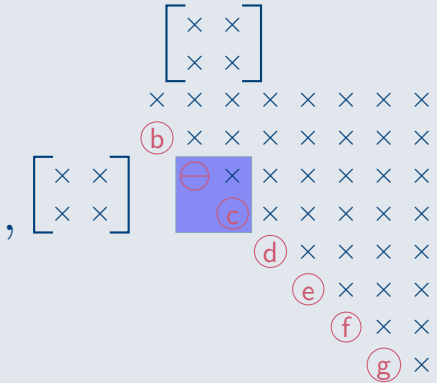

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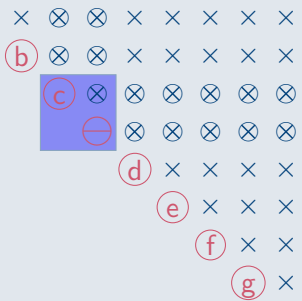

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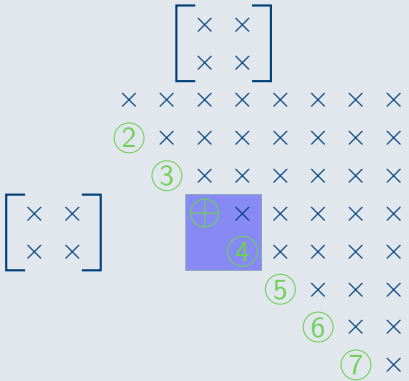

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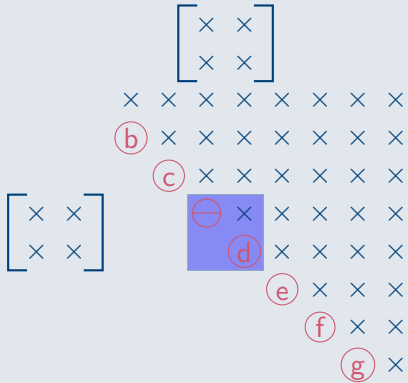

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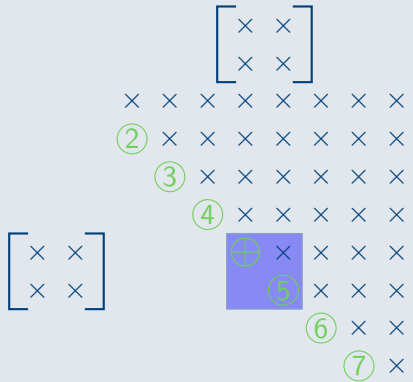

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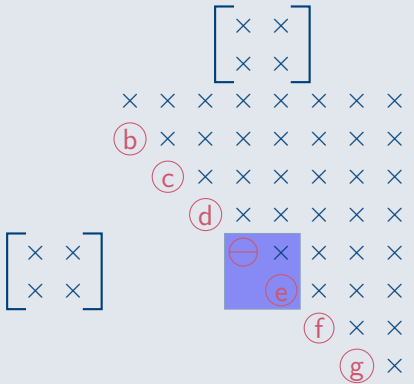

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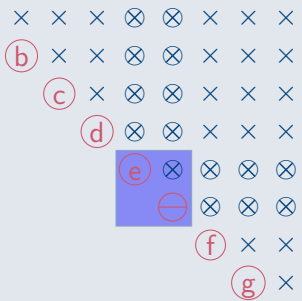

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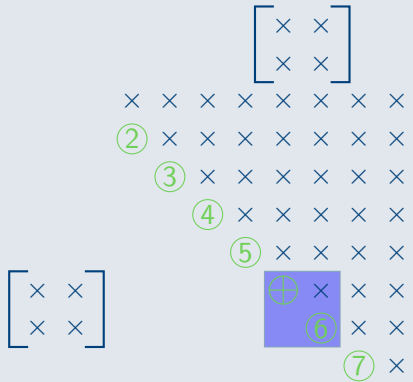

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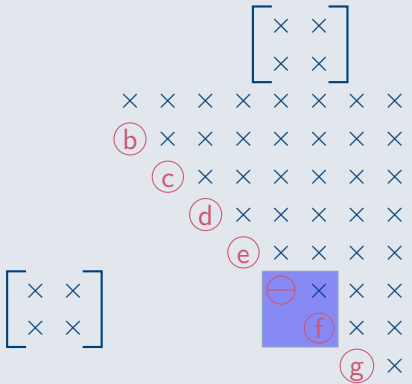

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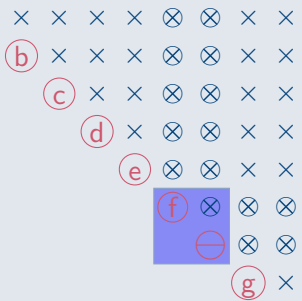

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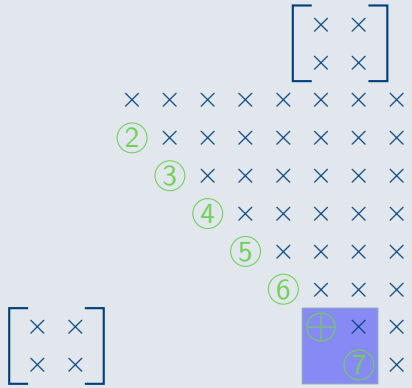

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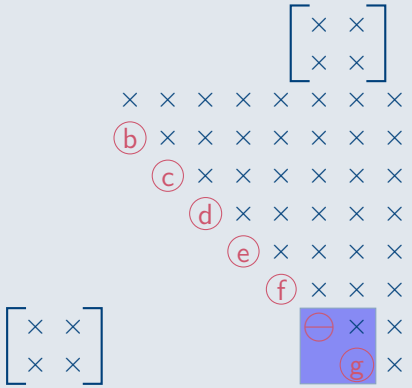

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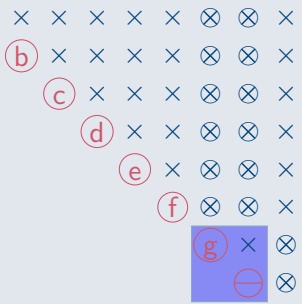

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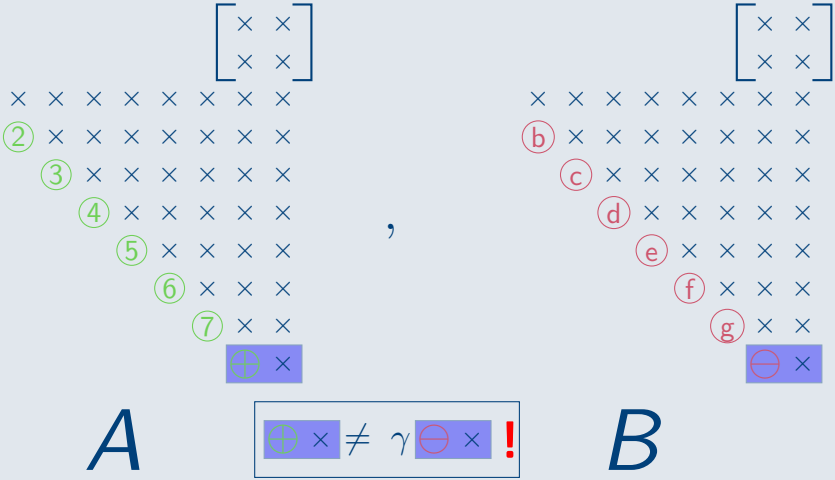
Changing the last pole/Removing the shift



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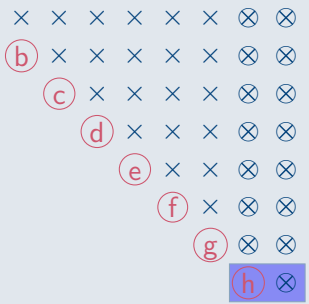

B

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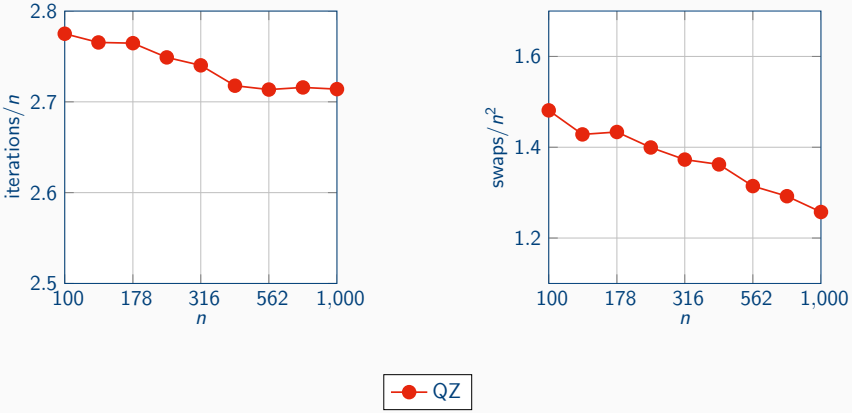
Poles at ∞ ($\times = 0$) $\rightarrow$ QZ method: Bulge exchange interpretation [Watkins]

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

Numerical example

Is it worth it?

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



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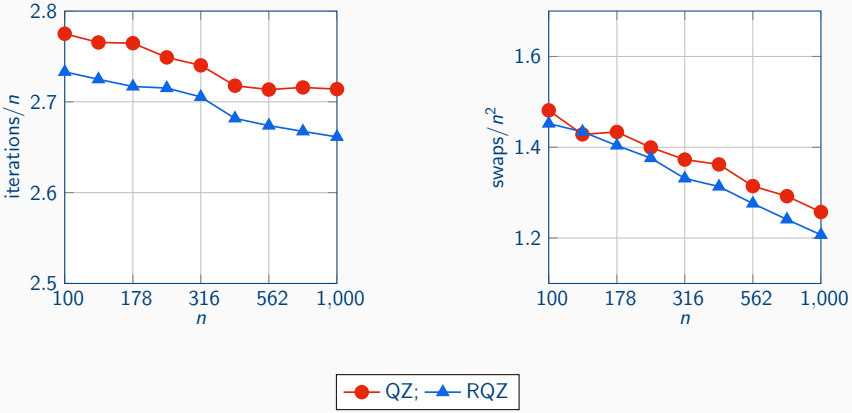

$\Rightarrow$ up to $5 - 10\%$ reduction in iterations with obvious choice of poles.

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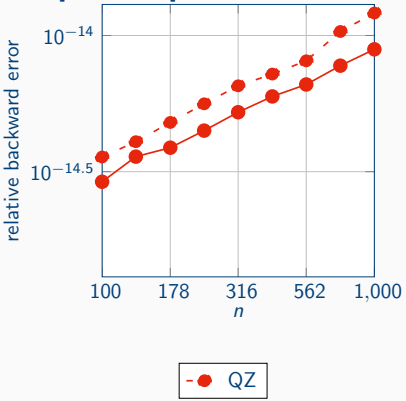

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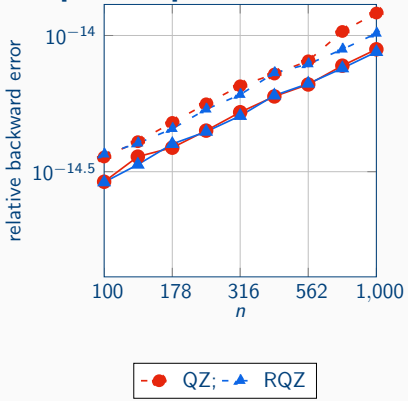


Reduction to Hessenberg form with poles Ξ

Step 1: QR factorization of B

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

Reduction to Hessenberg form with poles Ξ

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

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

Reduction to Hessenberg form with poles Ξ

Step 3: Restore upper triangularity of B

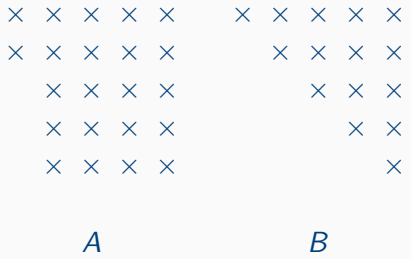
$A \leftarrow AZ_4$ $B \leftarrow BZ_4$

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



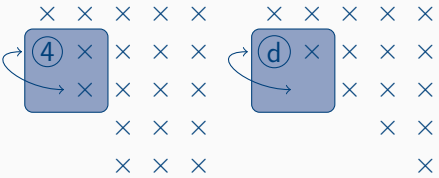
Reduction to Hessenberg form with poles Ξ

Step 7: Change first pole to ξ_{n-1}

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

Reduction to Hessenberg form with poles Ξ

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 ∞

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

Reduction to Hessenberg form with poles Ξ

Step 10: Change first pole to ξ_{n-2}

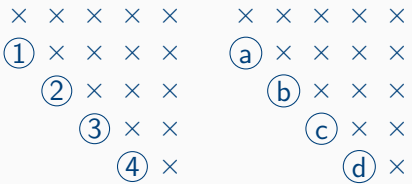
$A \leftarrow Q_1^* A$ $\qquad$ $B \leftarrow Q_1^* B$

Reduction to Hessenberg form with poles Ξ

... Continue with this process until...

Reduction to Hessenberg form with poles Ξ

End result



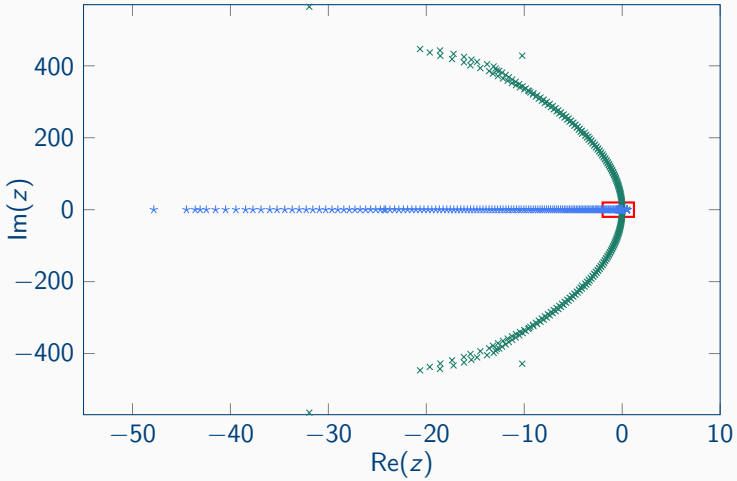
Reduction to Hessenberg form with poles Ξ

Computational cost:

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

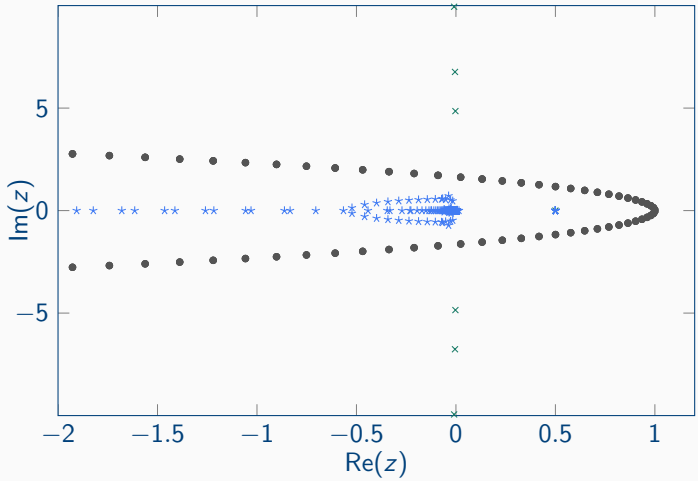
Numerical example: Reduction to Hessenberg form

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



Numerical example: Reduction to Hessenberg form

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



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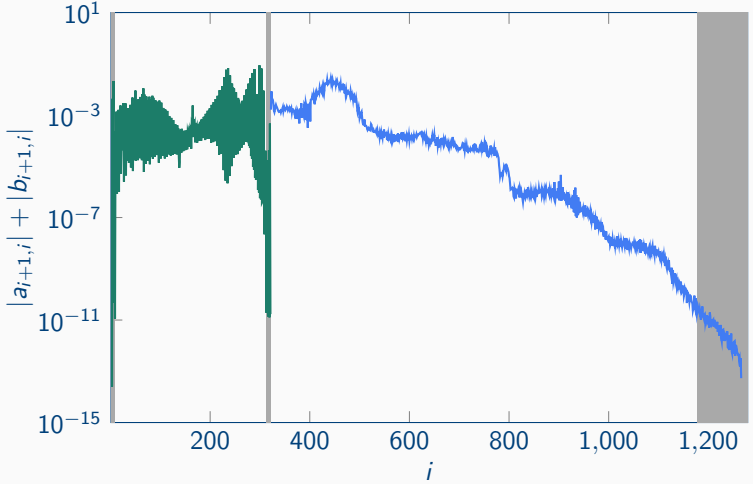
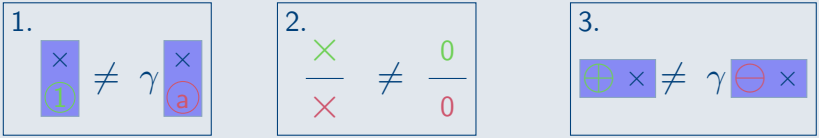


A word on the theory

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

$$\mathcal{R}(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_i) = (A - \varrho B)(A - \xi_i B)^{-1}\, \mathcal{E}_i$$
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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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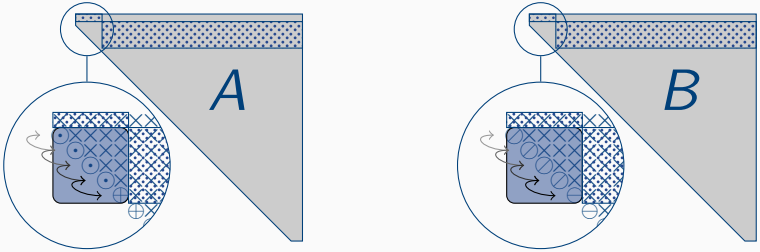
What does this mean?

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

Further extensions

Tightly packed shifts



→ More cache efficient implementations (Level 3 BLAS)

Further extensions

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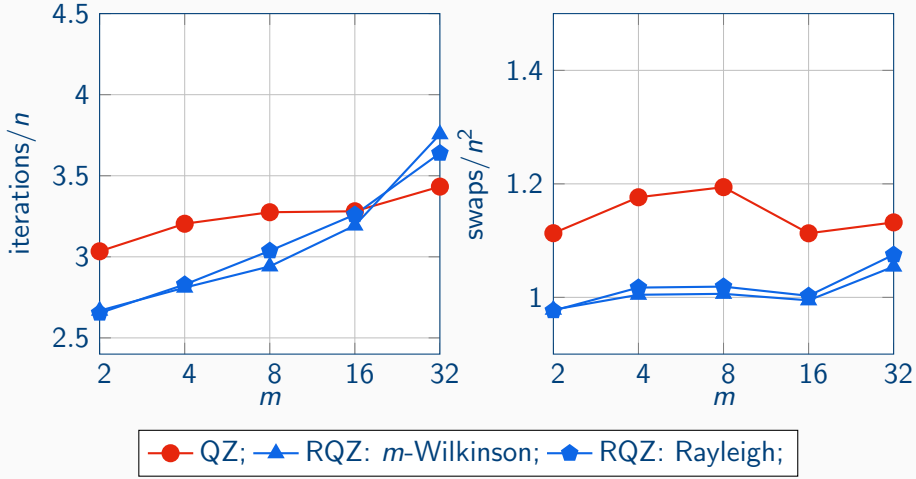
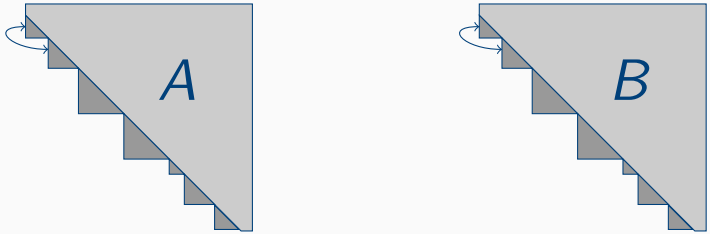


Further extensions

Block Hessenberg

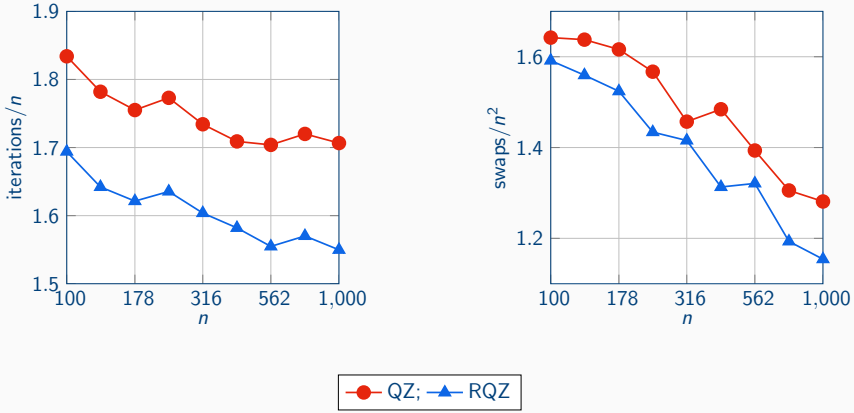


$\rightarrow$ complex conjugate shifts and poles in real arithmetic for real pencils

Further extensions

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!