KU LEUVEN

RQZ: A rational QZ method for the generalized eigenvalue problem

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

Overview

In this talk 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
- ◊ Subspace iteration

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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 a *manageable* form
  2. Iterate to generalized Schur form
  3. Recover eigenvectors
- Make use of well-chosen unitary equivalences:

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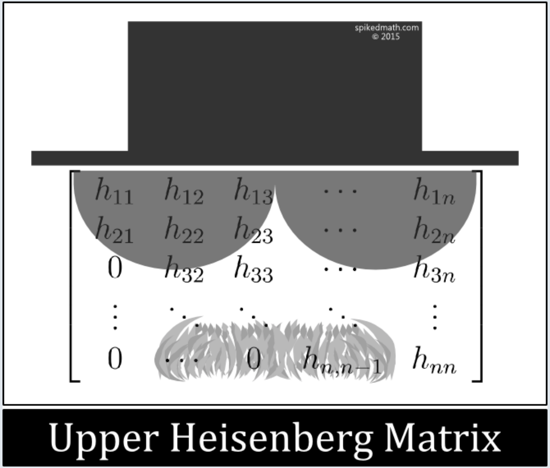
Hessenberg, Hessenberg form



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Hessenberg, Hessenberg form

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\underset{B}{\begin{matrix}
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\end{matrix}}
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Tools

Hessenberg, Hessenberg form

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 & & & & & & \times & \times
\end{matrix}}_{B}
$$

Tools

Hessenberg, Hessenberg form

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

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

$$\text{poles } \Xi = \left(\frac{\color{green}{\times}}{\color{red}{\times}}\right) \subset \bar{\mathbb{C}}$$

Hessenberg, Hessenberg form

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\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 \\
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\end{matrix}
\quad , \quad
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\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}
$$

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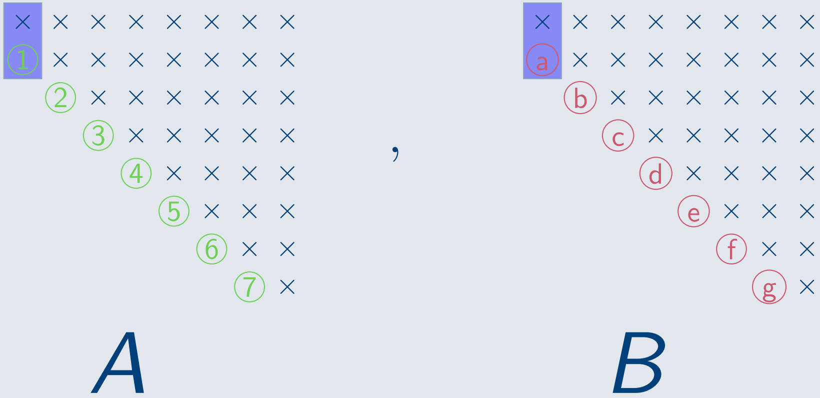
Tools

Introducing a shift



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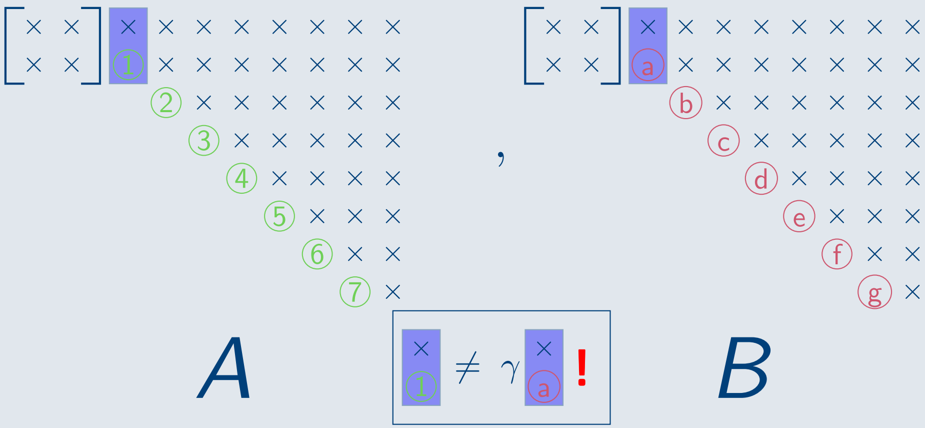

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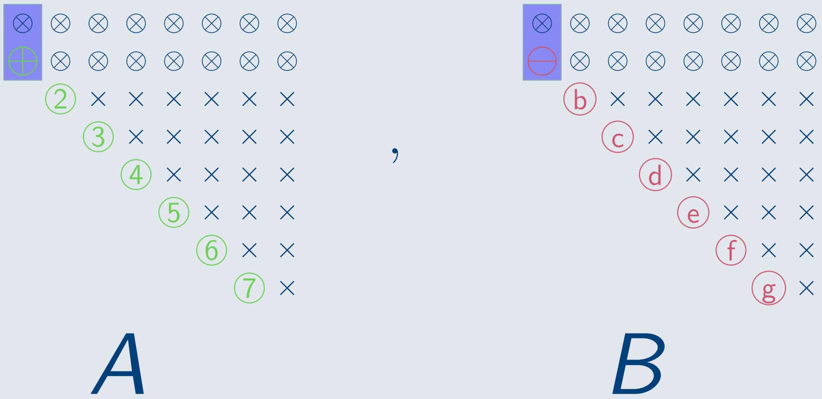

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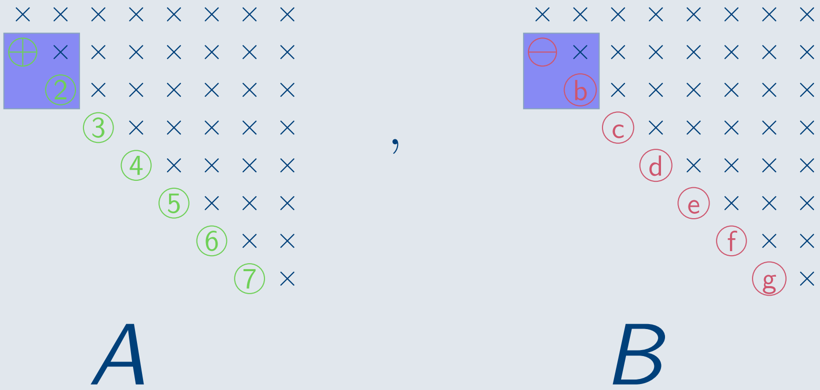
Swapping poles



Swapping poles

Solve coupled Sylvester equation

(cfr. reordering Schur form [Kågström and Poromaa])

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

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

Tools

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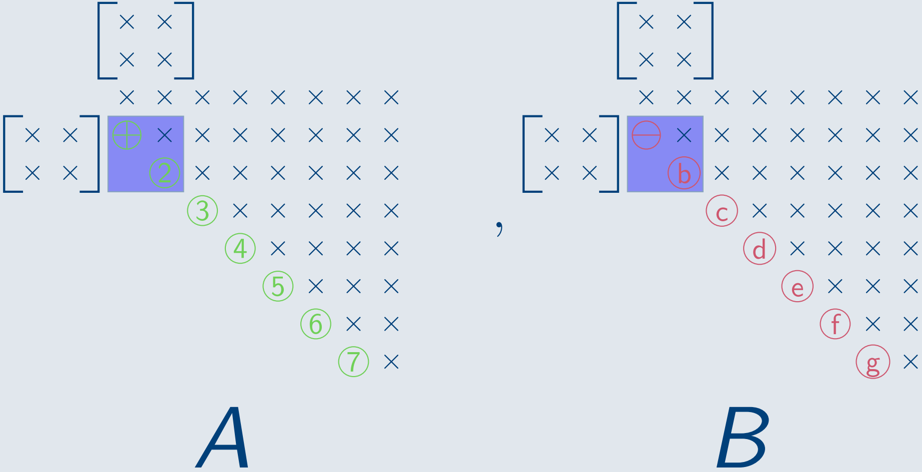

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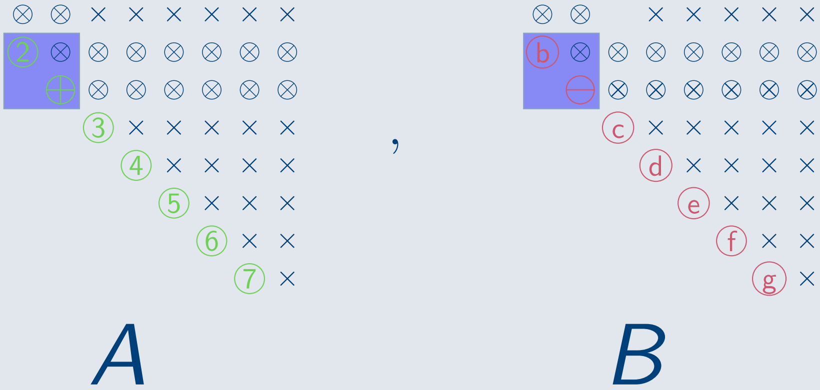

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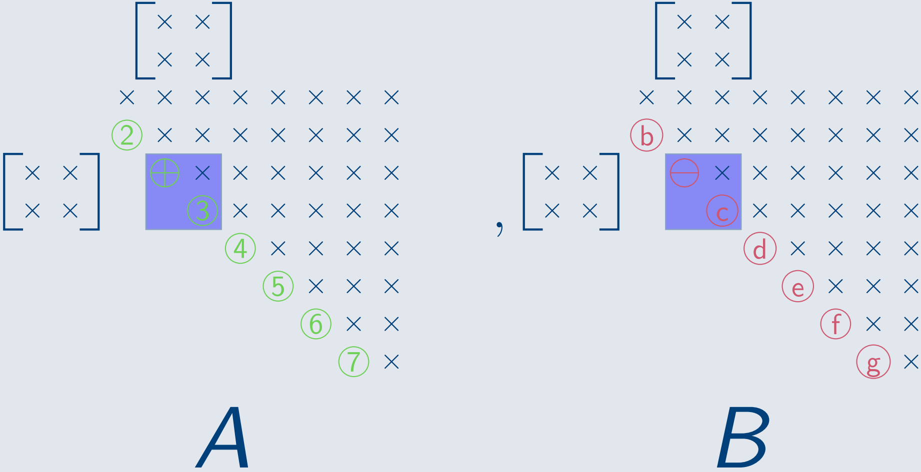

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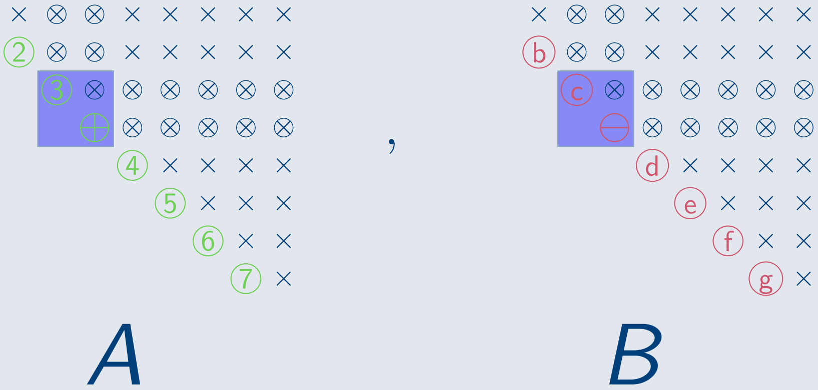

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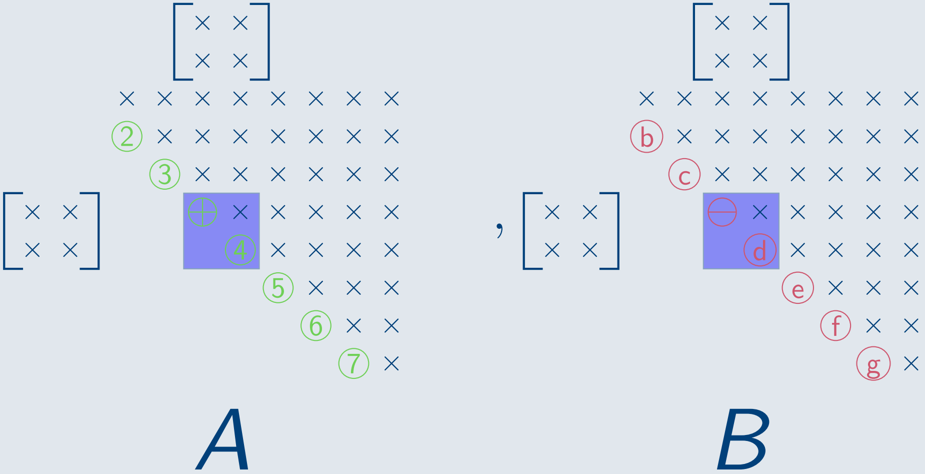

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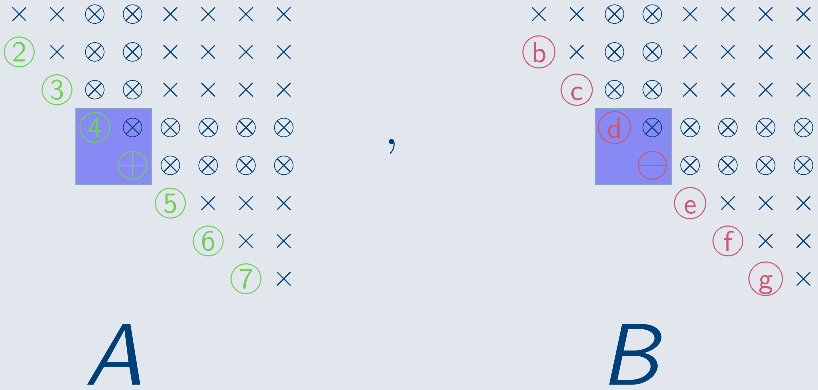

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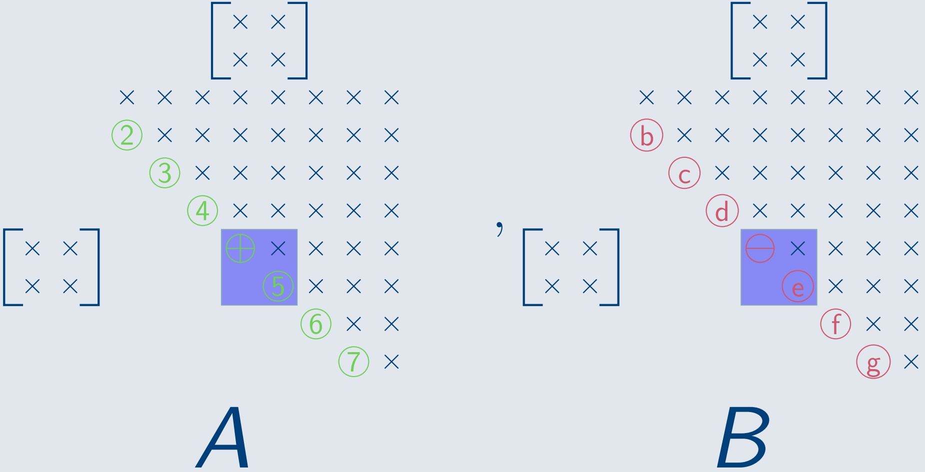

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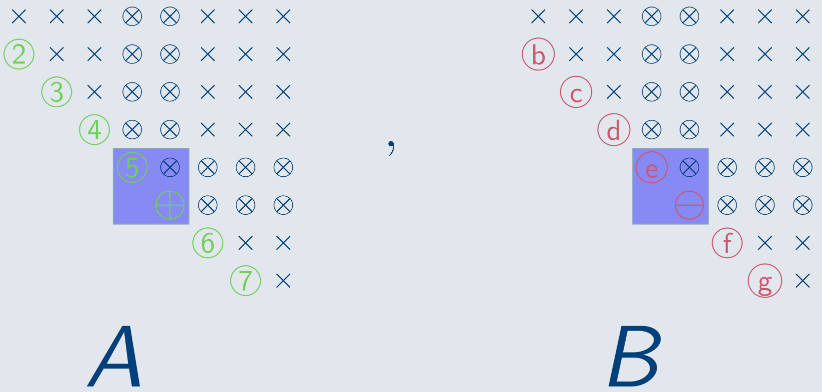

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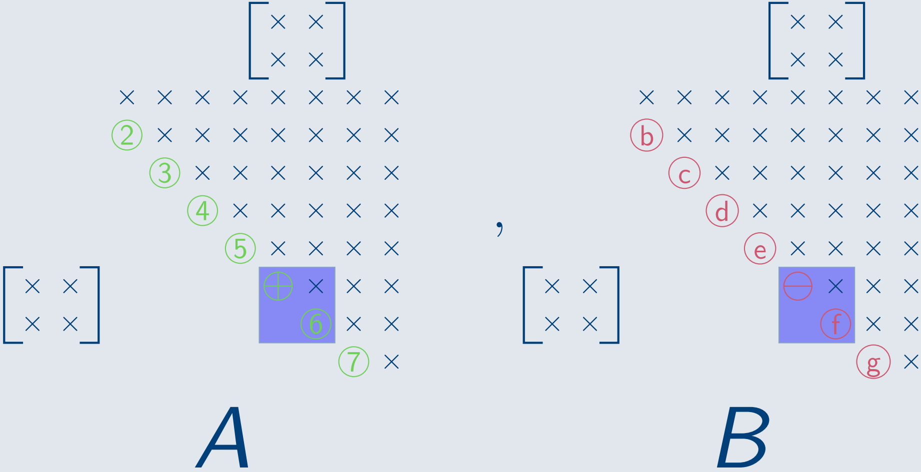

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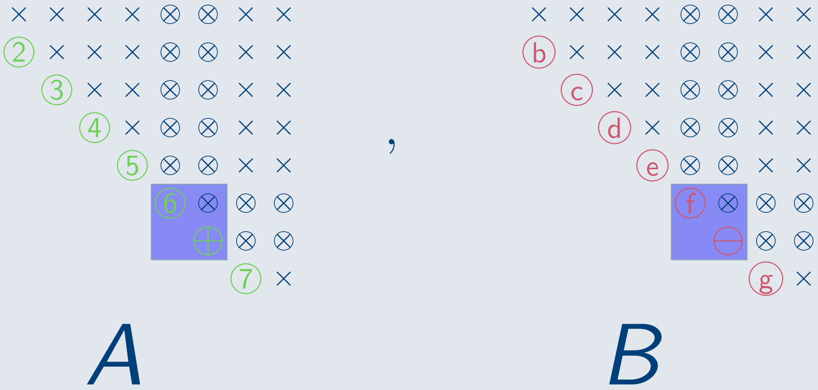

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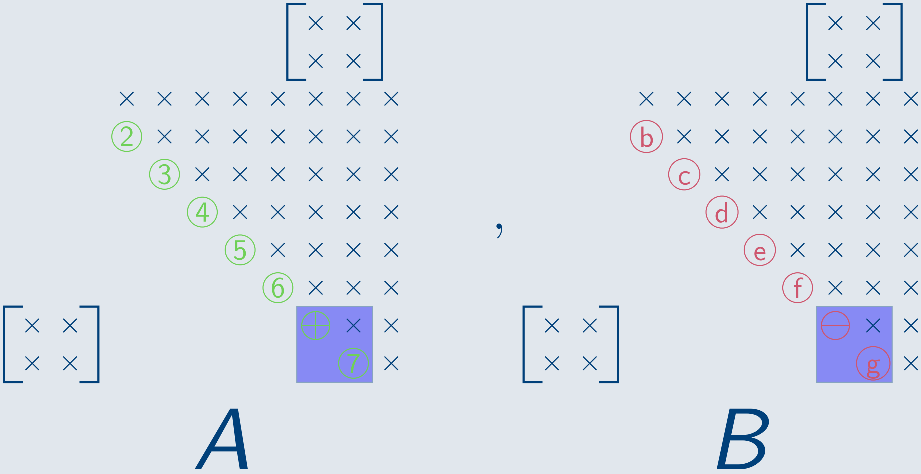

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Swapping poles

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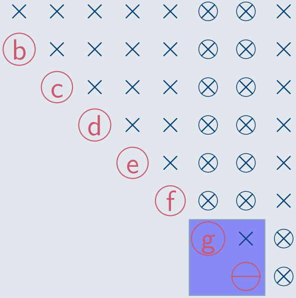
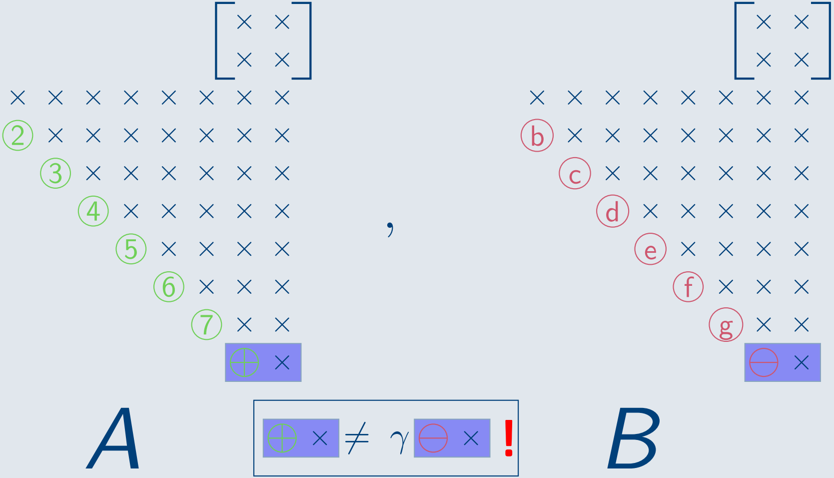


B

Tools

Introducing a pole



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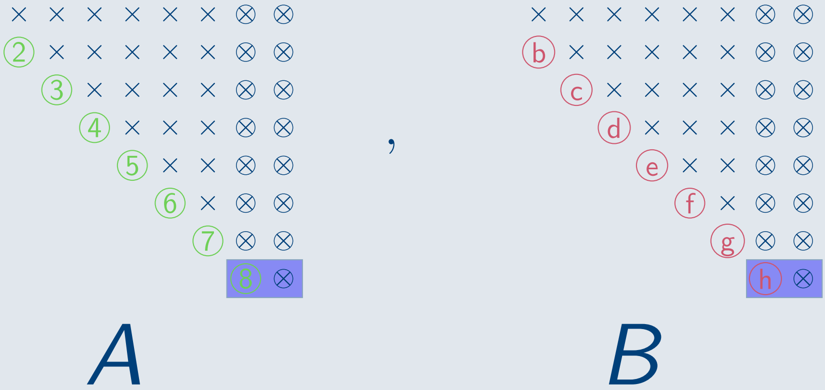

The algorithm in a nutshell:

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1. Introduce shift at the top

RQZ algorithm

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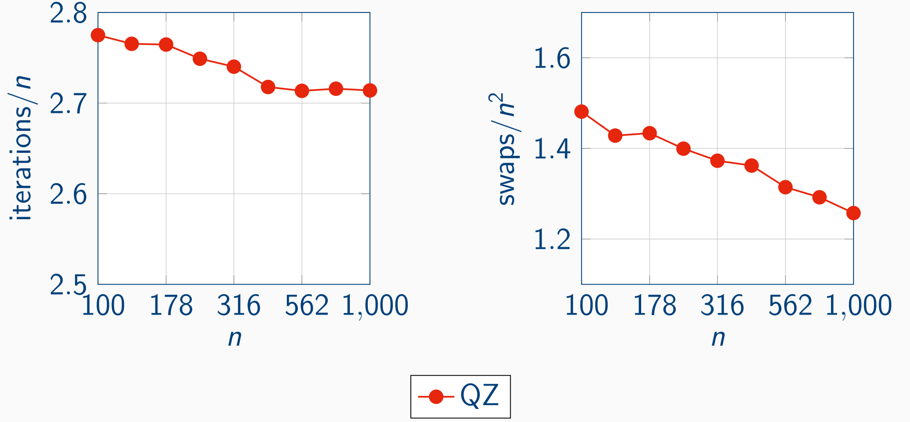
Poles at ∞ **(**$\times = 0$**)** $\rightarrow$ **QZ method**: Bulge exchange interpretation [Watkins]

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

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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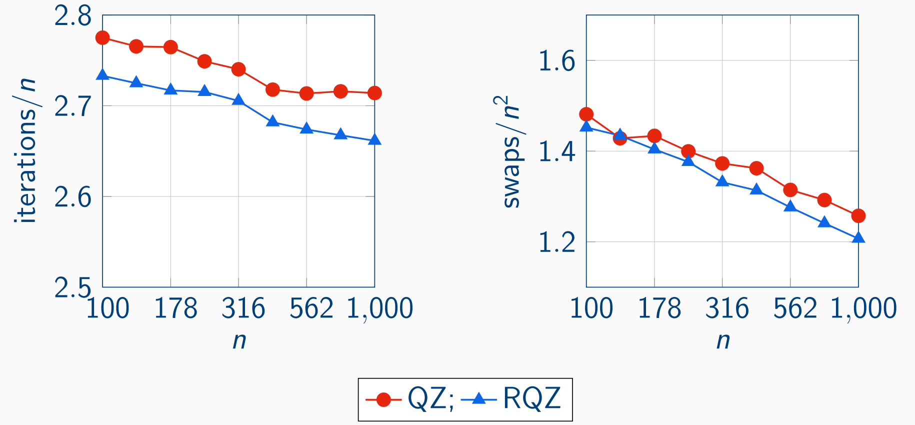

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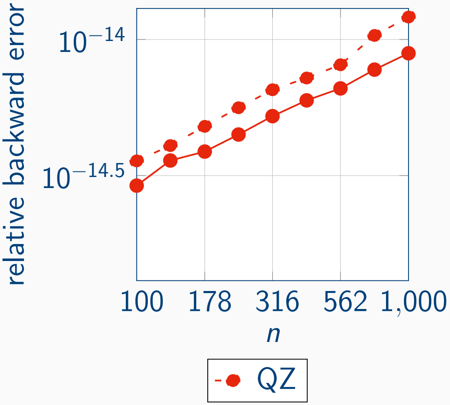

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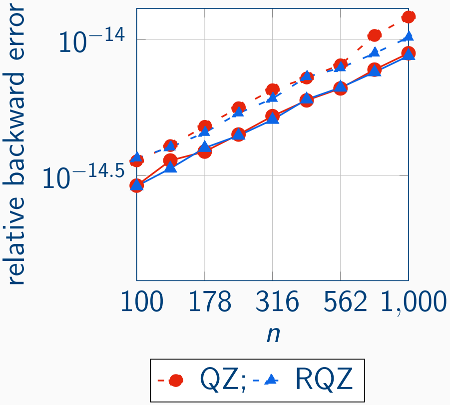

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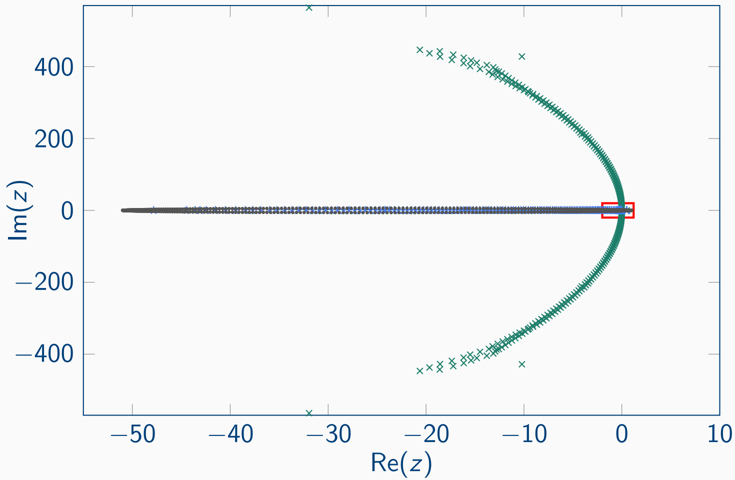
Numerical example 2: Reduction to Hessenberg, Hessenberg

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



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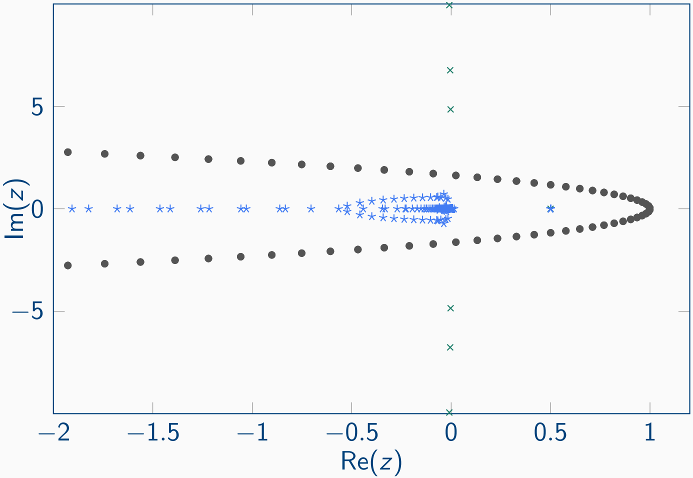

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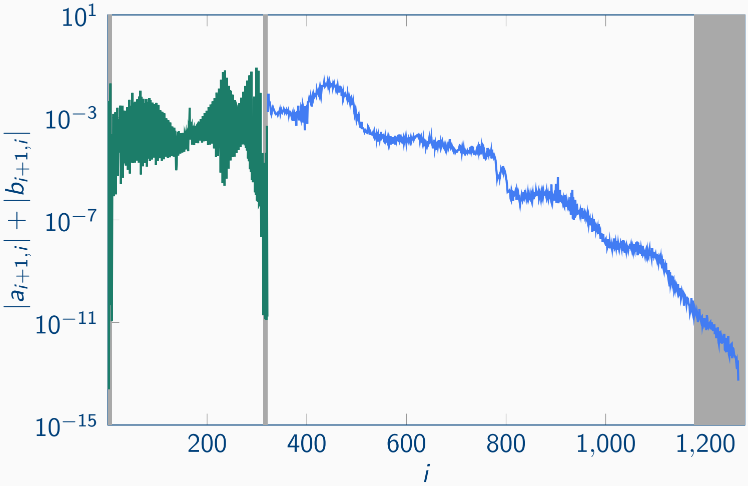
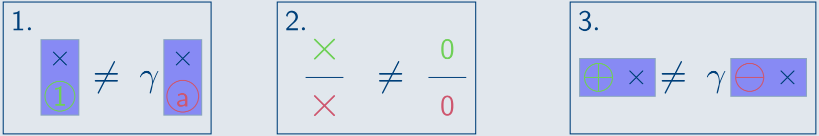


A word on the theory

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 $(\xi_1, \dots, \xi_{n-1})$ then for $i = 1, \dots, n-1$:

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

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 pencil with poles $(\xi_1, \dots, \xi_{n-1})$ and new pole ξ_n performs nested subspace iteration for $i = 1, \dots, n-1$ accelerated by

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

A word on the theory

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What does this mean?

- QR step with shift ϱ on entire space

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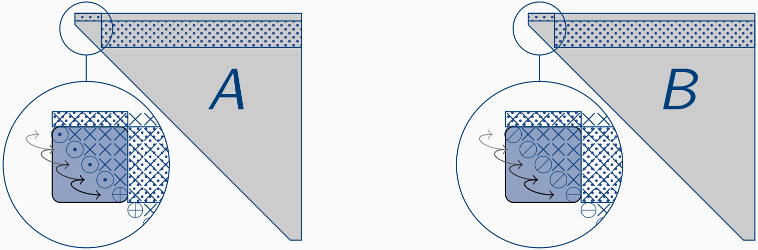
What does this mean?

- QR step with shift ϱ on entire space
- RQ steps with tightly packed shifts Ξ on selected subspaces

Further extensions

Tightly packed shifts



→ More cache efficient implementations (Level 3 BLAS)

Further extensions

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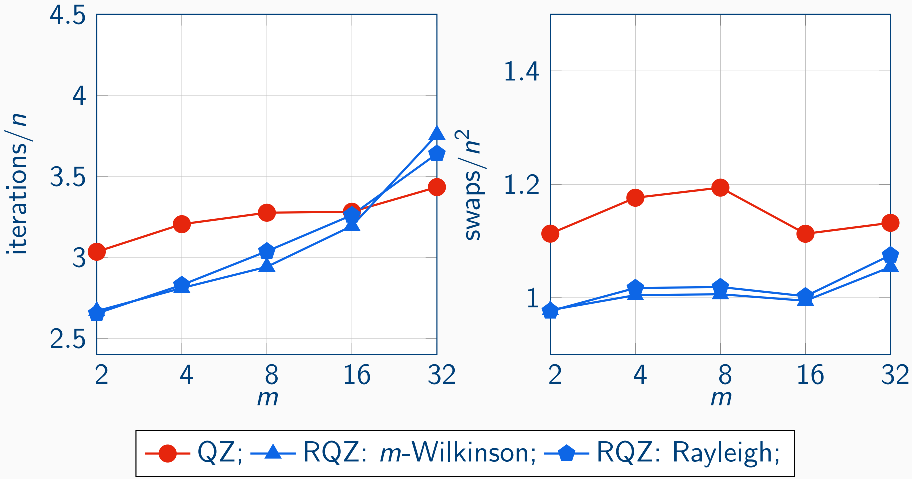
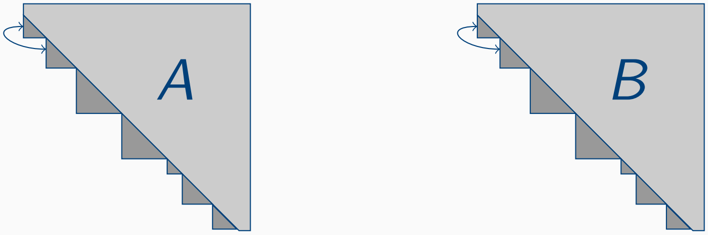


Further extensions

Block Hessenberg



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

Further extensions

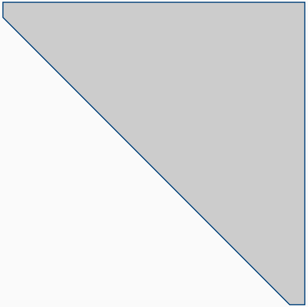
Aggressive Early deflation

The performance of the QR algorithm can be significantly improved by an aggressive early deflation technique ([Braman, Byers and Mathias]) and similar techniques have been developed for the QZ method ([Kågström and Kressner]).

Further extensions

Aggressive Early deflation

A and B



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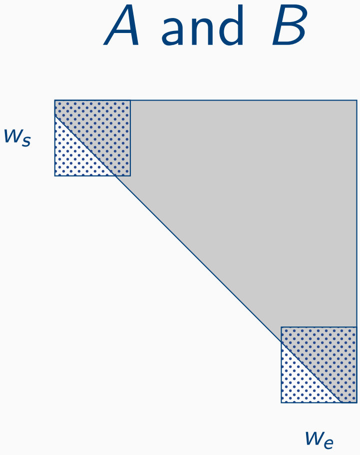

$n \gg w_e > w_s$

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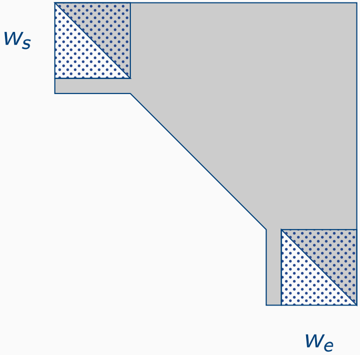

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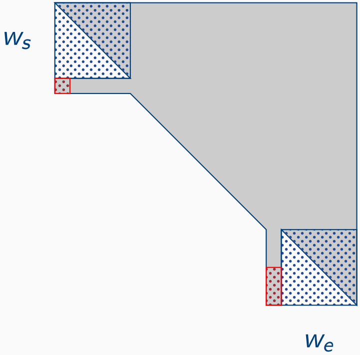

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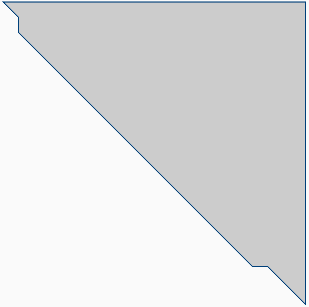

Further extensions

Standard eigenvalue problems

- RQZ applies equivalence transformations on the pencil:

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

- Consequently we have two similarity transformations:

$$\hat{A}\hat{B}^{-1} = Q^*AB^{-1}Q \quad \text{and} \quad \hat{B}^{-1}\hat{A} = Z^*B^{-1}AZ$$

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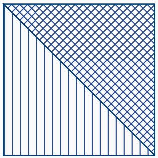

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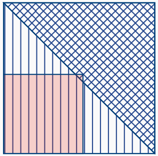

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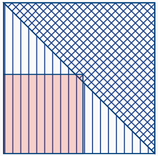

Extended Hessenberg + diagonal = rational Hessenberg

→ my connection with this mini-symposium

Extensions

Rational Krylov method

The connection between RQZ and the rational Krylov method can be used:

- to compute the Ritz values from the Hessenberg, Hessenberg recurrence pencil
- to filter and restart the rational Krylov method

Extensions

Rational Krylov method

$$A\, V_{k+1}\, \underline{G}_k = B\, V_{k+1}\, \underline{H}_k$$

with:

- $\mathcal{R}(V_{k+1}) = \mathcal{K}^{\text{rat}}_{k+1}(AB^{-1}, \boldsymbol{v}, \Xi_{1:k})$
- $(\underline{H}_k, \underline{G}_k)$ the Hessenberg, Hessenberg recurrence pencil

Applying an RQZ step with shift ϱ, we get $\mathcal{K}^{\text{rat}}_{k}(AB^{-1}, \hat{\boldsymbol{v}}, \Xi_{2:k})$ with:

$$\hat{\boldsymbol{v}} = (A - \xi_1\, B)^{-1}(A - \varrho\, B)\, \boldsymbol{v}$$

Conclusions

1. RQZ is a generalization of QZ
2. Implicit rational subspace iteration is promising
3. New shift and pole strategies can be a powerful tool to compute invariant subspaces

Further reading:

arXiv:1802.04094

`http://numa.cs.kuleuven.be/software/rqz/`

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Thank you for your attention!