Pole swapping methods for the eigenvalue problem

Rational QR algorithms

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- Paul Van Dooren
- Thomas Mach
- David Watkins
- Nicola Mastronardi

Overview

Introduction

Generalized eigenvalue problems

- Let $A, B \in \mathbb{F}^{n \times n}$ define a *matrix pair* (A, B) or *matrix pencil* $A - \lambda B$.
- Regular: $\det(A - \lambda B) \neq 0$.
- Generalized eigenvalue problem:

$$A\boldsymbol{x} = \lambda B\boldsymbol{x}, \quad \lambda \in \bar{\mathbb{C}} := \mathbb{C} \cup \{\infty\}.$$

Generalized eigenvalue problems

- For a regular matrix pencil $A - \lambda B$ there exists unitary matrices Q and Z such that

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

  with $S - \lambda T$ upper triangular and $\Lambda(A, B) = \{s_{11}/t_{11}, s_{22}/t_{22}, \ldots\}$.
- The QZ method (Moler-Stewart, 1973) is the default algorithm to compute the generalized Schur decomposition.

Bulge chasing

- The QZ method generalizes the QR method of (Francis, 1961-62) for the standard eigenvalue problem
- It is a bulge chasing algorithm which consists out of two phases:
  1. Initial (direct) reduction to equivalent Hessenberg, upper triangular form

$$H - \lambda R = Q^*(A - \lambda B)Z$$

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

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

Bulge chasing

Bulge chasing =

- Motivated by implicit Q theorems
  $\Rightarrow$ iterates are uniquely determined by $\boldsymbol{q}_1 = p(AB^{-1})\boldsymbol{e}_1$
- Nested subspace iteration with a change of basis accelerated by polynomials (shifts) (Elsner-Watkins, 1991; Watkins, 1993)

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

Pole swapping

Rational Krylov

Polynomial	Rational
Krylov subspace $\mathcal{K}_{m+1}(A, \boldsymbol{v}) := \mathcal{R}(\boldsymbol{v}, A\boldsymbol{v}, \ldots, A^m \boldsymbol{v})$	**rational Krylov subspace** $\mathcal{K}^{\text{rat}}_{m+1}(A, \boldsymbol{v}, \Xi) := q(A)^{-1}\mathcal{K}_{m+1}(A, \boldsymbol{v})$ • $\Xi = (\xi_1, \ldots, \xi_m) \subset \bar{\mathbb{C}} \setminus \Lambda$ • $q(z) = \prod_{\xi_i \neq \infty}(z - \xi_i)$
Arnoldi Decomposition (Arnoldi, 1951) $AV_m = V_{m+1}\underline{H}_m$	**rational Arnoldi** (Ruhe, 1998) $AV_{m+1}\underline{K}_m = V_{m+1}\underline{L}_m$ • $\ell_{i+1,i}/k_{i+1,i} = \xi_i$
Uniqueness $\boldsymbol{v}$ fixed $\Leftrightarrow (V_{m+1}, \underline{H}_m)$ unique	**Uniqueness** (Berljafa-Güttel, 2015) $\boldsymbol{v}$ and Ξ fixed $\Leftrightarrow (V_{m+1}, \underline{K}_m, \underline{L}_m)$ unique

Rational Krylov

Berljafa-Güttel (2015)

Two methods to change the poles in a rational Arnoldi decomposition

$$A V_{m+1} \underline{K}_m = V_{m+1} \underline{L}_m$$

- Implicitly by changing $\boldsymbol{v}_1$
- Explicitly by pole swapping

$\Rightarrow$ Equivalent if $\mathcal{R}(V_{m+1})$ is fixed.

C.-Meerbergen-Vandebril (2019a)

The pole swapping technique can be used as a direct method for the eigenvalue problem: rational QZ algorithm.

Rational QZ

Hessenberg pencils

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\end{matrix}}_{B}
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Hessenberg pencils

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

Rational QZ

Hessenberg pencils

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\begin{array}{cccccccc}
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\textcircled{a} & \times & \times & \times & \times & \times & \times & \times \\
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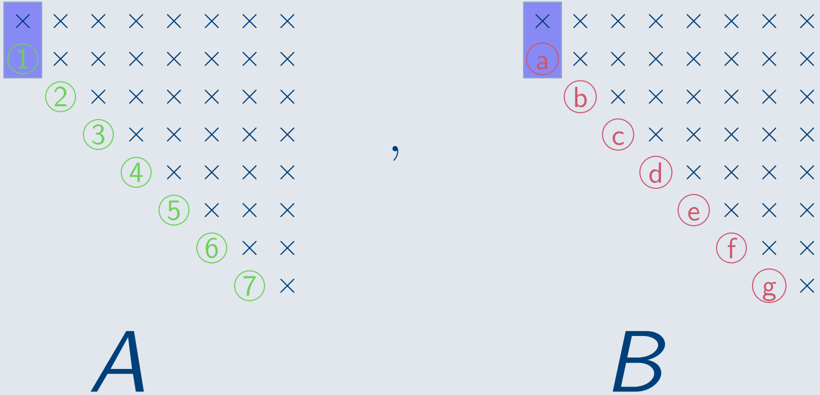
 & & & \textcircled{d} & \times & \times & \times & \times \\
 & & & & \textcircled{e} & \times & \times & \times \\
 & & & & & \textcircled{f} & \times & \times \\
 & & & & & & \textcircled{g} & \times
\end{array}
$$

$$A \qquad\qquad B$$

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

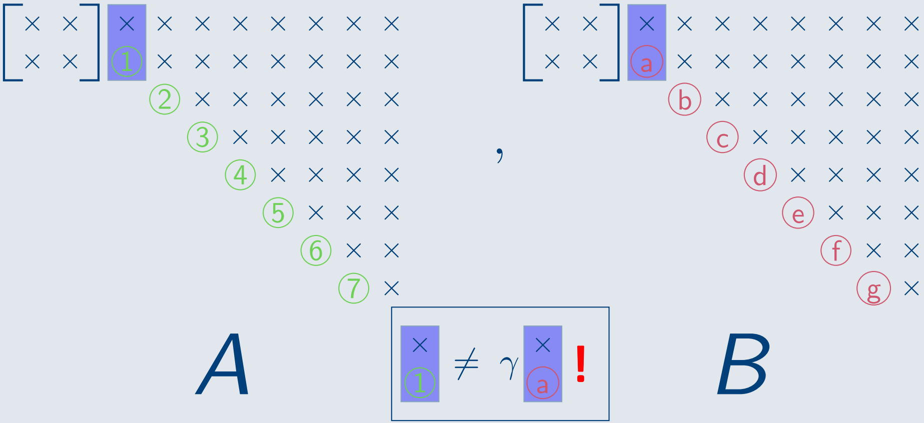
Rational QZ: an example

Introducing a shift



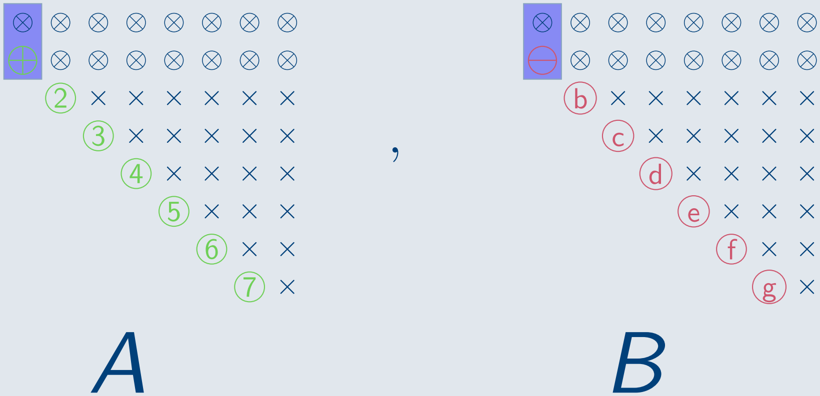
Rational QZ: an example

Introducing a shift



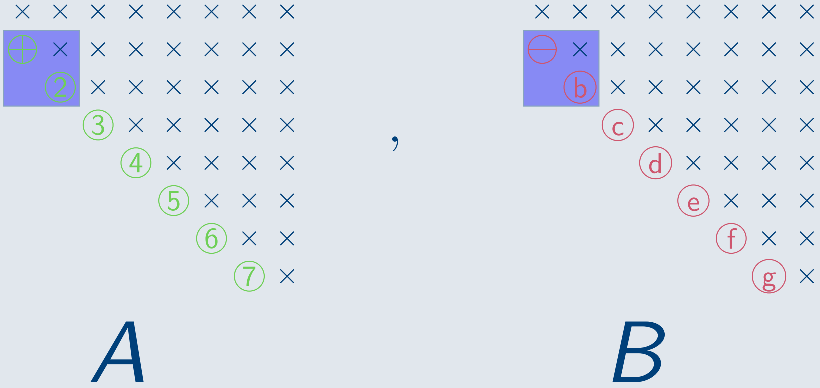
Rational QZ: an example

Introducing a shift



Rational QZ: an example

Swapping poles



Rational QZ: an example

Swapping poles

Classical problem in NLA:

Reordering generalized Schur form

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

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

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

Rational QZ: an example

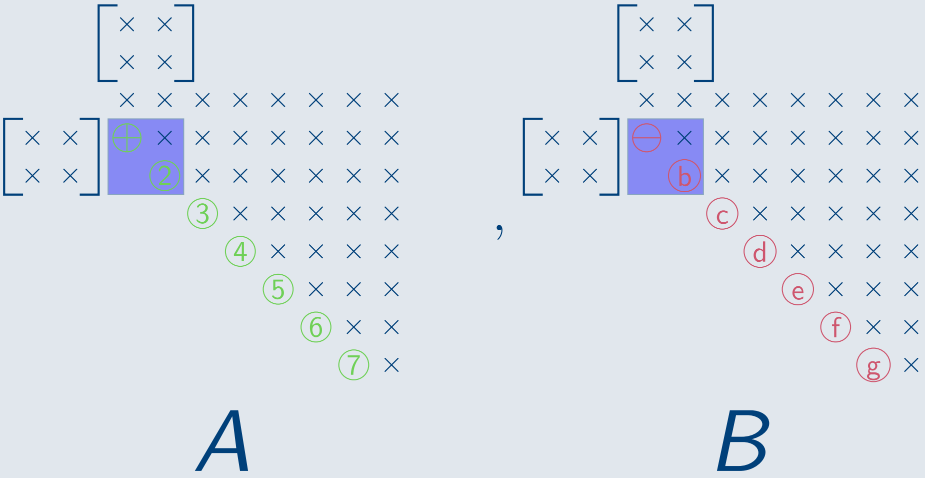
Swapping poles

Table 1: Distribution of errors $\hat{a}_{21}/\|A\|$ and $\hat{b}_{21}/\|B\|$ for our method, Van Dooren's method, and the Sylvester method.

$\hat{x}_{21}/\|X\|$		$[0, 10^{-16}]$	$(10^{-16}, 10^{-15}]$	$(10^{-15}, 10^{-10}]$	$(10^{-10}, 10^{-5}]$	$(10^{-5}, 10^{0}]$
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%

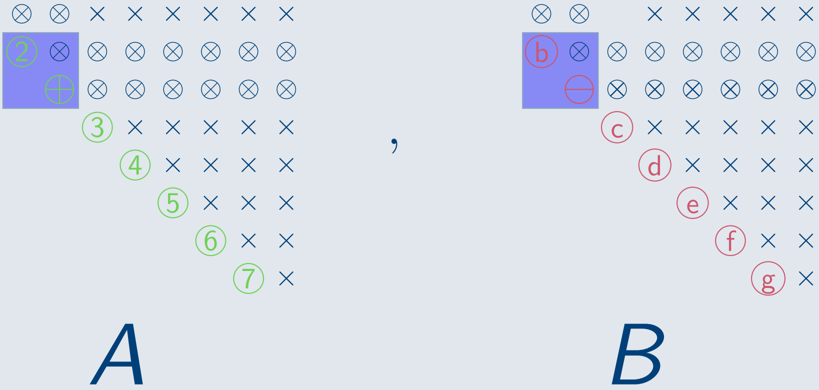
Rational QZ: an example

Swapping poles



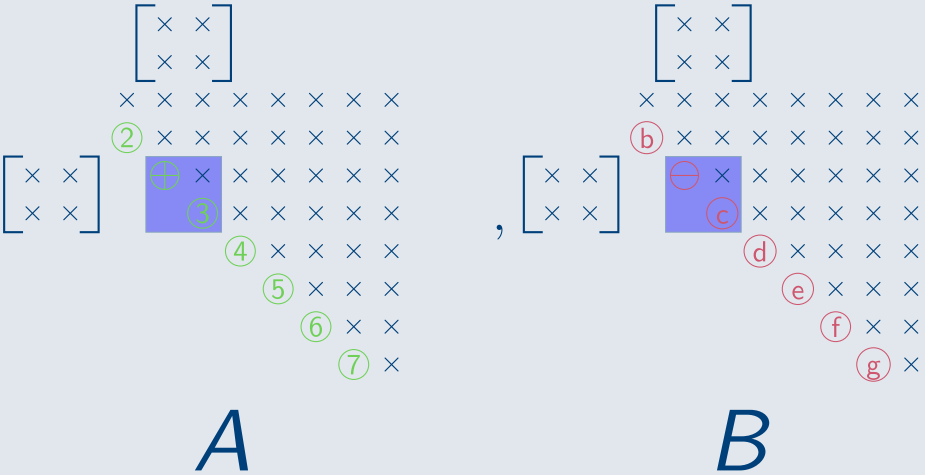
Rational QZ: an example

Swapping poles



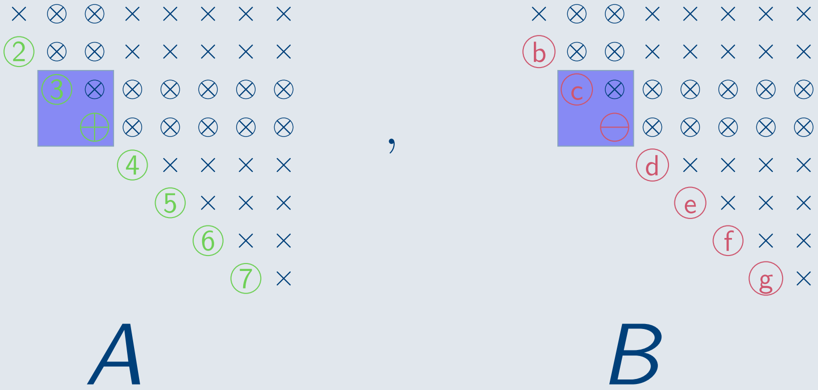
Rational QZ: an example

Swapping poles



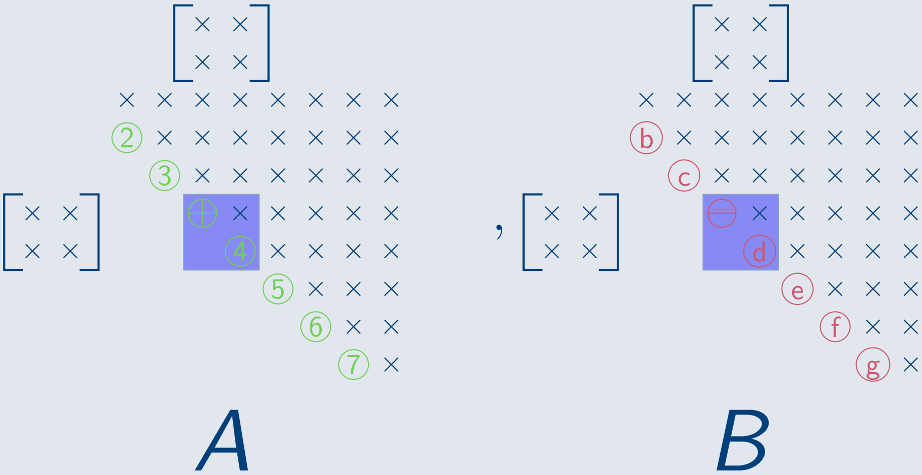
Rational QZ: an example

Swapping poles



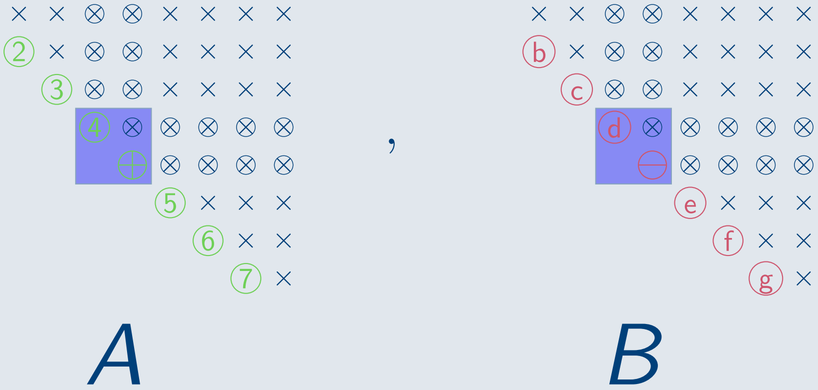
Rational QZ: an example

Swapping poles



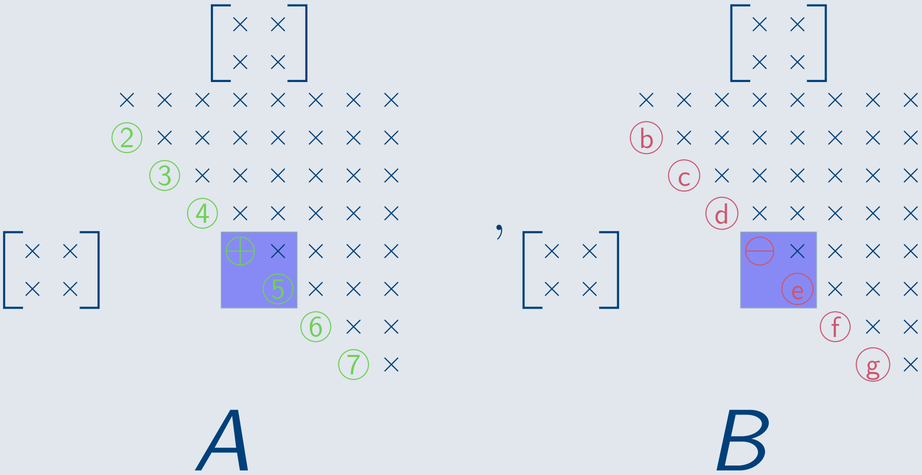
Rational QZ: an example

Swapping poles



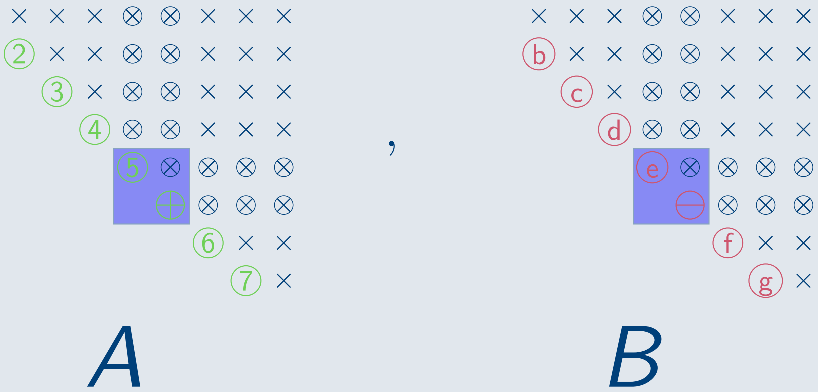
Rational QZ: an example

Swapping poles



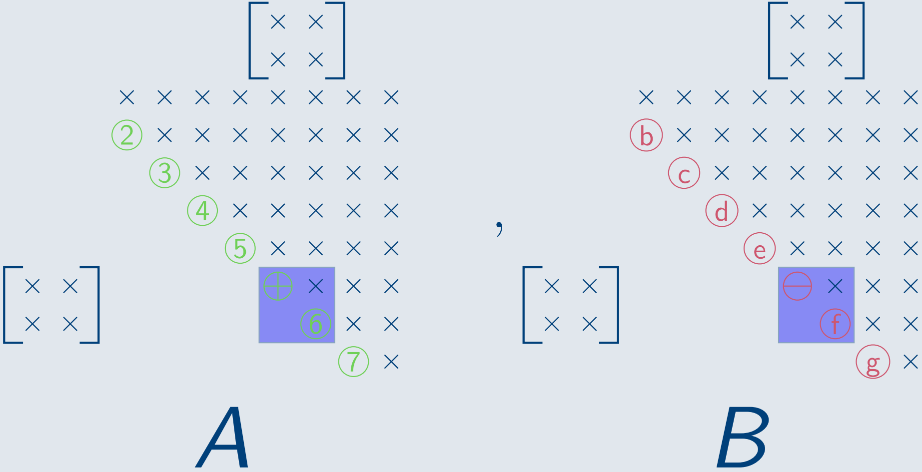
Rational QZ: an example

Swapping poles



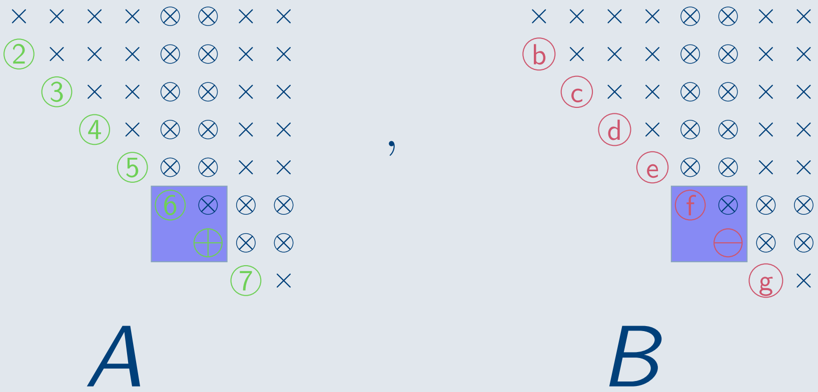
Rational QZ: an example

Swapping poles



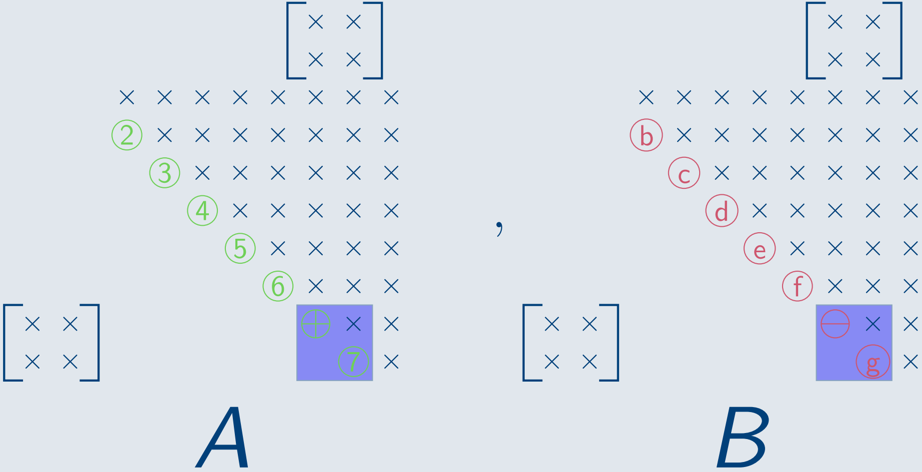
Rational QZ: an example

Swapping poles



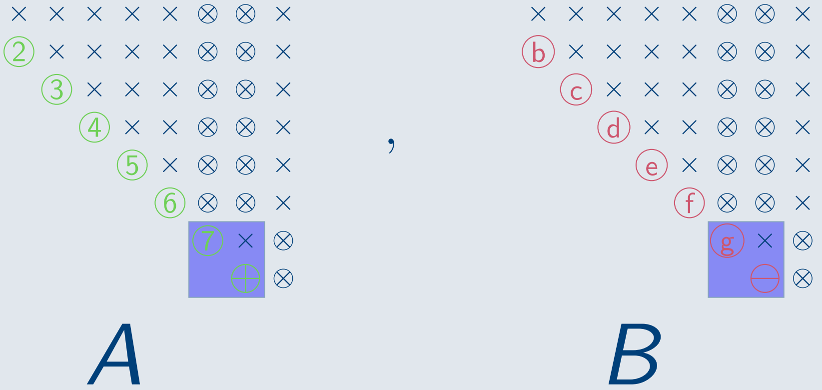
Rational QZ: an example

Swapping poles



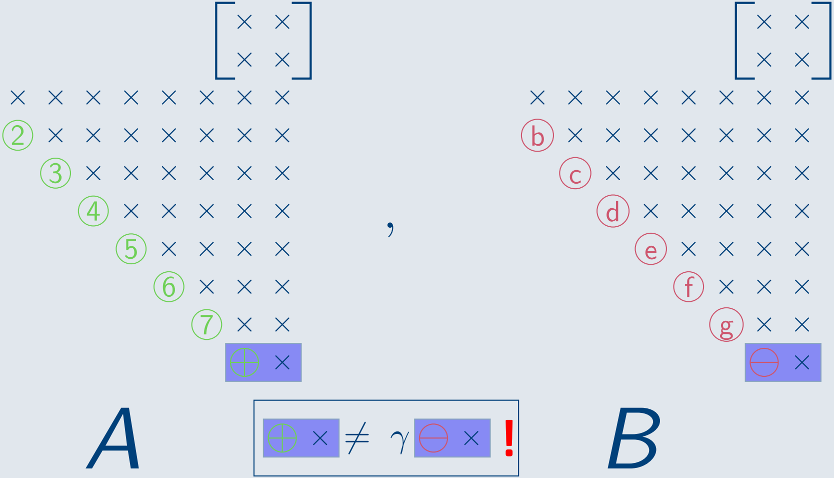
Rational QZ: an example

Swapping poles



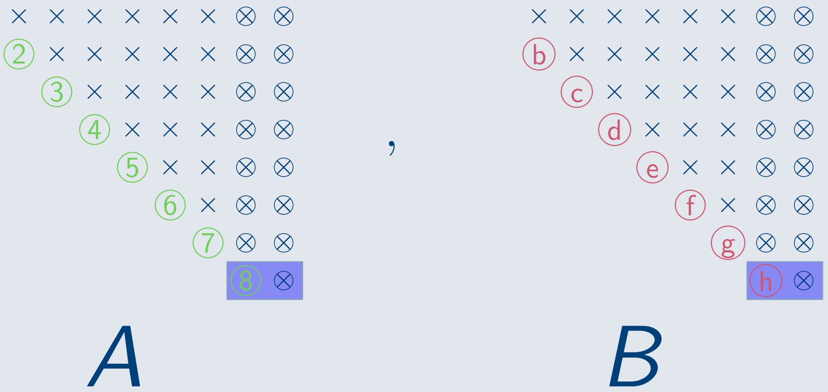
Rational QZ: an example

Introducing a pole



Rational QZ: an example

Introducing a pole



Classical QZ as a special case

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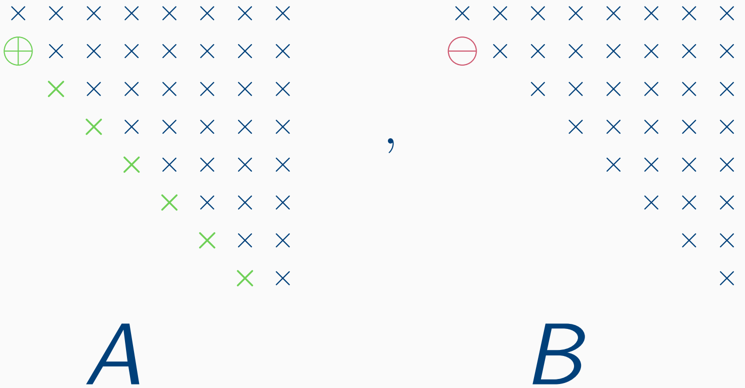
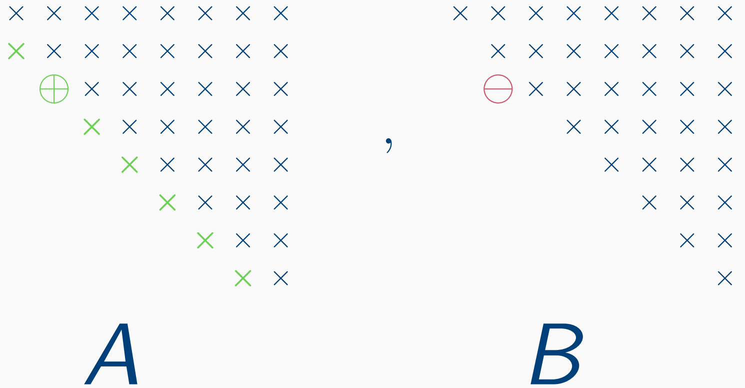
$$A \qquad\qquad\qquad B$$

Classical QZ as a special case



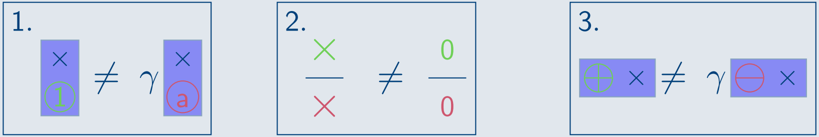
Classical QZ as a special case



Theoretical results

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

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

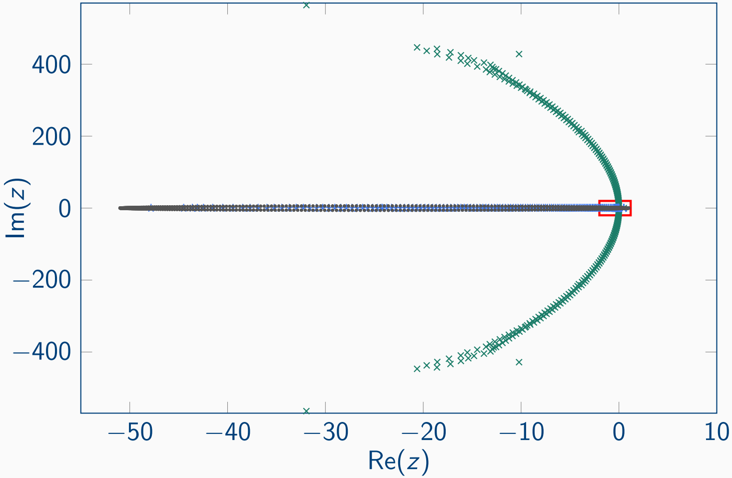
Pole swapping =

- 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

Numerical example: Reduction to Hessenberg form

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



Numerical example: Reduction to Hessenberg form

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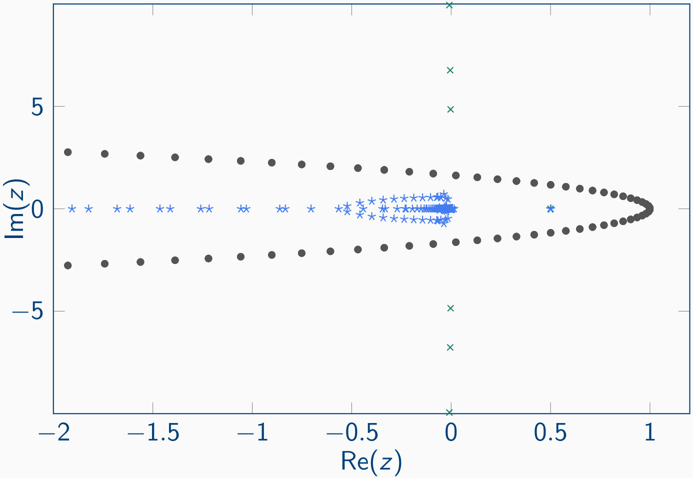

Numerical example: Reduction to Hessenberg form

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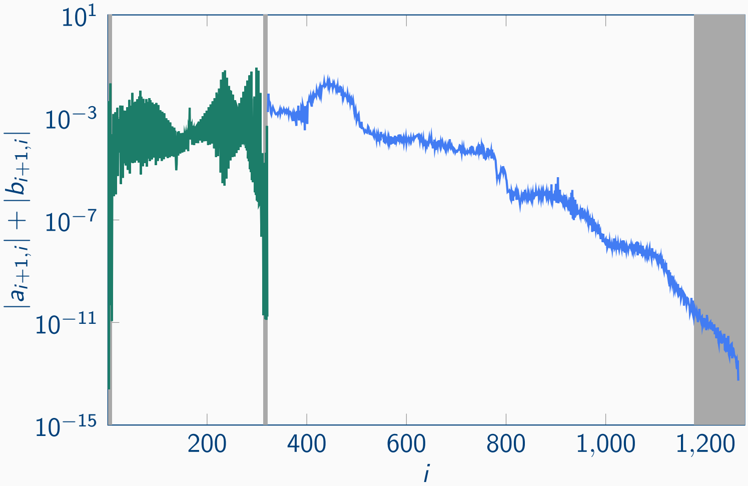


Multishift, multipole rational QZ

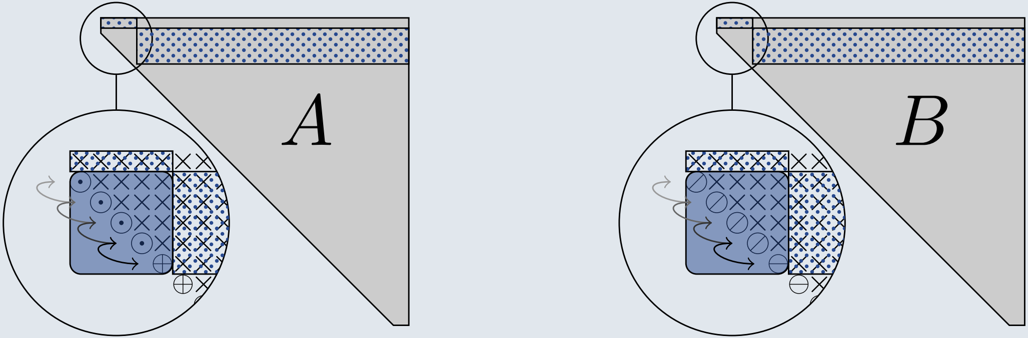
Multishift, multipole rational QZ

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 (C.-Mastronardi-Vandebril-Van Dooren, 2019).

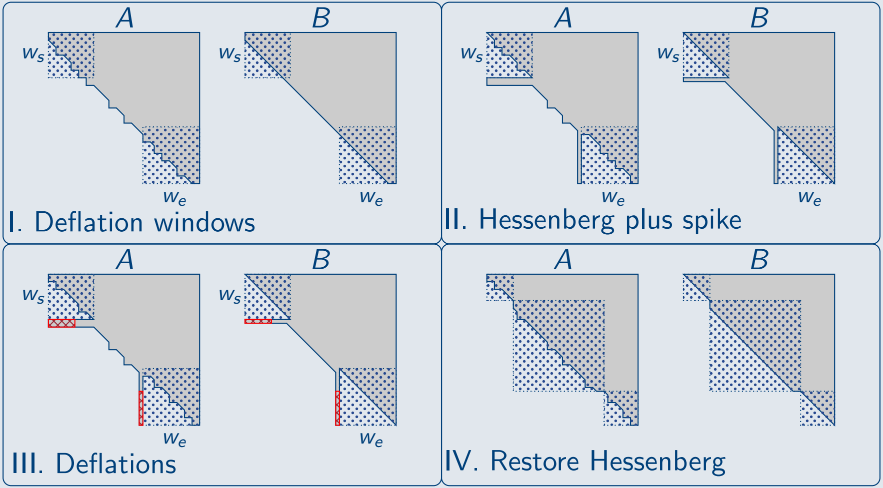
Multishift, multipole rational QZ

Batched operations



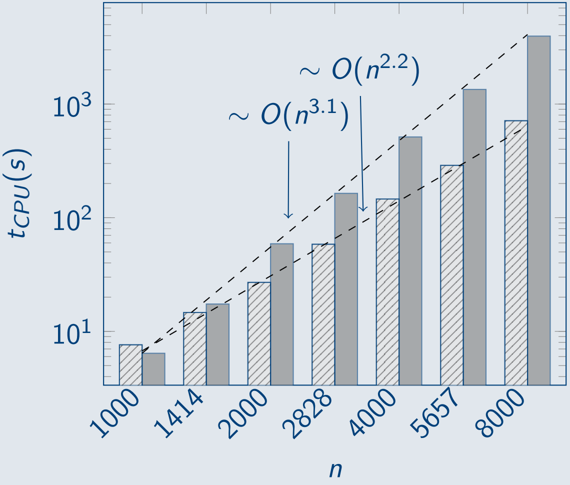
Multishift, multipole rational QZ

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



Multishift, multipole rational QZ

Numerical experiments with `libRQZ v0.1`



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.

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