Rational matrix algorithms for the generalized eigenvalue problem

Iterative and direct methods

Daan Camps, Karl Meerbergen, and Raf Vandebril

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

Overview

Part I

Standard eigenvalue problem

Large scale: Polynomial Krylov

$\updownarrow$

Medium scale: Francis' *QR* algorithm

Part II

Generalized eigenvalue problem

Large scale: Rational Krylov

$\updownarrow$

Medium scale: Rational *QZ* algorithm

Part I: Polynomial methods

Standard eigenvalue problem (SEP)

Definition SEP

- $A \in \mathbb{C}^{n \times n}$
- $(\lambda, \boldsymbol{x})$ is called an *eigenpair* of A if

$$A\boldsymbol{x} = \lambda \boldsymbol{x}.$$

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<u>Assume:</u> 1 GHz CPU $\rightarrow 10^9$ flop/s

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Polynomial Krylov methods for the SEP

Consider the sequence of $\ell + 1$ vectors:

$$\boldsymbol{v}, A\boldsymbol{v}, A^2\boldsymbol{v}, \dots, A^\ell\boldsymbol{v}.$$

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Assume $1 \leq \ell \leq n$ such that the vectors become linearly dependent.

Then

$$\exists p \in \mathcal{P}_\ell : p(A)\boldsymbol{v} = a_0\boldsymbol{v} + a_1 A\boldsymbol{v} + \ldots + a_\ell A^\ell \boldsymbol{v} = \boldsymbol{0} \qquad \text{with } a_\ell \neq 0$$

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If we factorize:

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Definition polynomial Krylov subspace

- $A \in \mathbb{C}^{n\times n}$ and $\boldsymbol{v} \in \mathbb{C}^n$
- The Krylov subspace of order $m+1$:

$$\mathcal{K}_{m+1}(A, \boldsymbol{v}) = \mathrm{span}\{\boldsymbol{v}, A\boldsymbol{v}, \dots, A^m\boldsymbol{v}\}$$

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Issue with $\mathcal{K}_{m+1}$

Assume $A = A^T \in \mathbb{R}^{n \times n}$. Suppose $|\lambda_1| > |\lambda_2|$ with eigenvector $\boldsymbol{x}_1$. Then

$$\|A^k \boldsymbol{v} - \boldsymbol{x}_1\| = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$$

.

$\Rightarrow$ this rapidly becomes a very ill-conditioned basis!

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Solution: create a basis of $\mathcal{K}_{m+1}$ with the best possible condition number ($= 1$)

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$m = 1$	$\mathcal{K}_2$	$\boldsymbol{v}_1$	$h_{11} = \boldsymbol{v}_1^* A \boldsymbol{v}_1$	$h_{21}\boldsymbol{v}_2 = A\boldsymbol{v}_1 - h_{11}\boldsymbol{v}_1$

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$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$m = k$	$\mathcal{K}_{k+1}$	$\boldsymbol{v}_1 \ \dots \ \boldsymbol{v}_k$	$\begin{aligned} h_{1k} &= \boldsymbol{v}_1^* A \boldsymbol{v}_k \\ &\ \vdots \\ h_{kk} &= \boldsymbol{v}_k^* A \boldsymbol{v}_k \end{aligned}$	$\begin{aligned} h_{k+1,k}\boldsymbol{v}_{k+1} = A\boldsymbol{v}_k - {} & h_{1k}\boldsymbol{v}_1 - \dots \\ - {} & h_{kk}\boldsymbol{v}_k \quad (\bigstar) \end{aligned}$

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At step k:

$$A\boldsymbol{v}_k = h_{1k}\boldsymbol{v}_1 + \ldots + h_{kk}\boldsymbol{v}_k + h_{k+1,k}\boldsymbol{v}_{k+1} \qquad (\star)$$

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Solution: create a basis of $\mathcal{K}_{m+1}$ with the best possible condition number $(= 1)$

At step k:

$$A\boldsymbol{v}_k = \begin{bmatrix} \boldsymbol{v}_1 & \dots & \boldsymbol{v}_k & \boldsymbol{v}_{k+1} \end{bmatrix} \begin{bmatrix} h_{1k} \\ \vdots \\ h_{kk} \\ h_{k+1,k} \end{bmatrix} \qquad (\bigstar)$$

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Combining all m steps:

$$A\, V_m = V_{m+1}\, \underline{H}_m$$

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Column/row k satisfies Eq. $(\bigstar)$

Polynomial Krylov methods for the SEP

How to extract eigenpairs from $\mathcal{K}_{m+1}$?

$\Rightarrow$ Compute the **Ritz pairs:**

$$H_m \boldsymbol{z} = \vartheta \, \boldsymbol{z}$$

Ritz pairs $(\vartheta, \boldsymbol{x}) \coloneqq (\vartheta, V_m \boldsymbol{z})$

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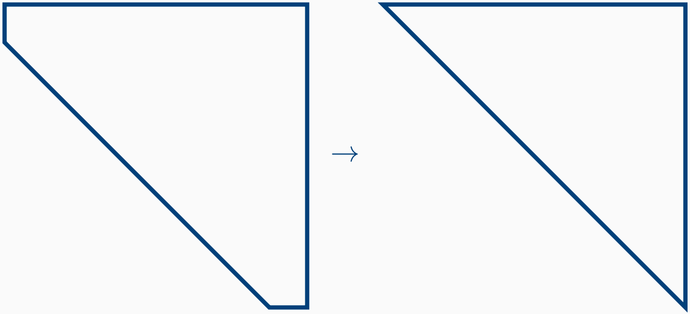
Link between iterative and direct methods

H_m upper Hessenberg matrix $\Rightarrow$ Francis' implicitly shifted QR

Implicitly shifted QR (Francis, 1961, 1962)

$$A \quad \to \quad \hat{A} = Q^* A Q$$



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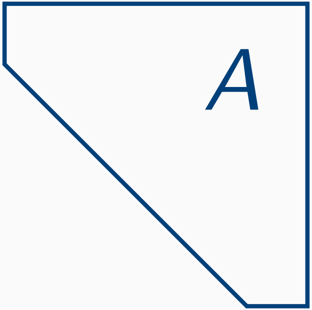

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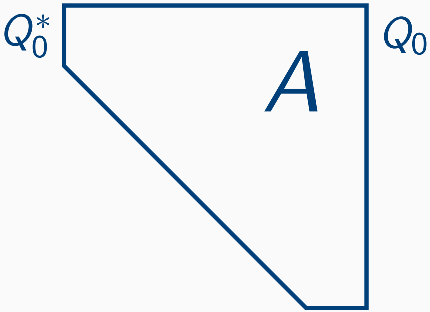

$$Q_0 \, \boldsymbol{e}_1 = \alpha(A - \varrho I)\boldsymbol{e}_1$$

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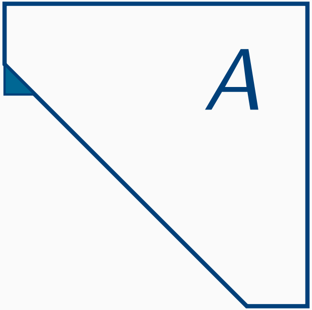

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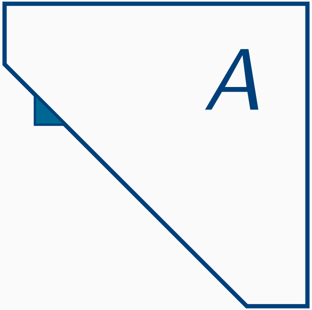

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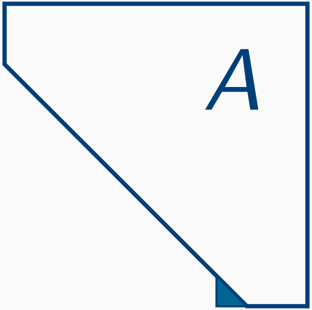

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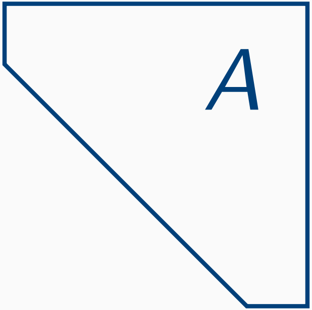

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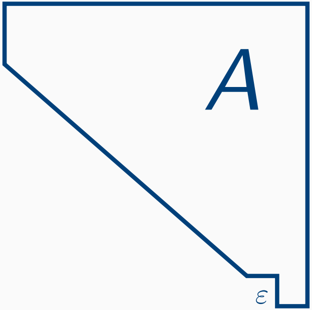


Part II: Rational methods

Generalized eigenvalue problem (GEP)

Definition GEP

- $A, B \in \mathbb{C}^{n \times n}$
- The triplet $(\alpha, \beta, \boldsymbol{x})$ is called an *eigentriplet* of (A, B) if:

$$\beta A\boldsymbol{x} = \alpha B\boldsymbol{x}.$$

Rational Krylov methods for the GEP

$A: \quad \mathcal{K}_{m+1} \;\Big|\; \boldsymbol{v}, A\boldsymbol{v}, \ldots, A^m\boldsymbol{v}$

Rational Krylov methods for the GEP

$$\begin{array}{rl|l} A: & \mathcal{K}_{m+1} & \boldsymbol{v}, A\boldsymbol{v}, \dots, A^m\boldsymbol{v} \\ (A,B): & \mathcal{K}_{m+1} & \boldsymbol{v}, B^{-1}A\boldsymbol{v}, \dots, (B^{-1}A)^m\boldsymbol{v} \end{array}$$

Rational Krylov methods for the GEP

$$
\begin{array}{rl|l}
A: & \mathcal{K}_{m+1} & \boldsymbol{v}, A\boldsymbol{v}, \ldots, A^m\boldsymbol{v} \\
(A,B): & \mathcal{K}_{m+1} & \boldsymbol{v}, B^{-1}A\boldsymbol{v}, \ldots, (B^{-1}A)^m\boldsymbol{v} \\
(A,B): & \mathcal{Q}_{m+1} & \boldsymbol{v}, M_1\boldsymbol{v}, \ldots, M_m\boldsymbol{w}
\end{array}
$$

The Möbius transformation of (A, B) with *pole* $\xi_i = -\beta_i/\alpha_i$ and zero $\varrho_i = -\delta_i/\gamma_i$:

$$M_i = (\alpha_i A + \beta_i B)^{-1}(\gamma_i A + \delta_i B) \tag{$\clubsuit$}$$

This leads to a subspace of *rational functions in* (A, B) with a fixed denominator.

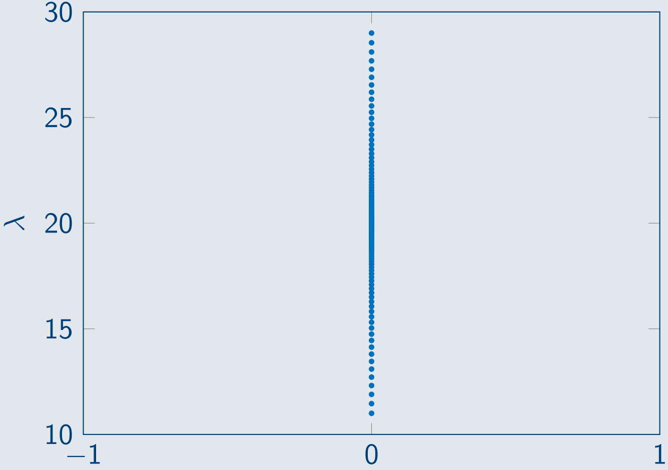
Rational Krylov methods for the GEP

Special choices for ($\clubsuit$) :

- *Polynomial Krylov:* $M = B^{-1}A$ with pole at $\xi = \infty$
- *Extended Krylov:* Either $\xi = \infty$ ($M = B^{-1}A$) or $\xi = 0$ ($M = A^{-1}B$)
- *Shift-and-invert Krylov:* A single, fixed ξ ($M = (A - \xi B)^{-1}B$)

Rational Krylov methods for the GEP

A short motivation for rational methods



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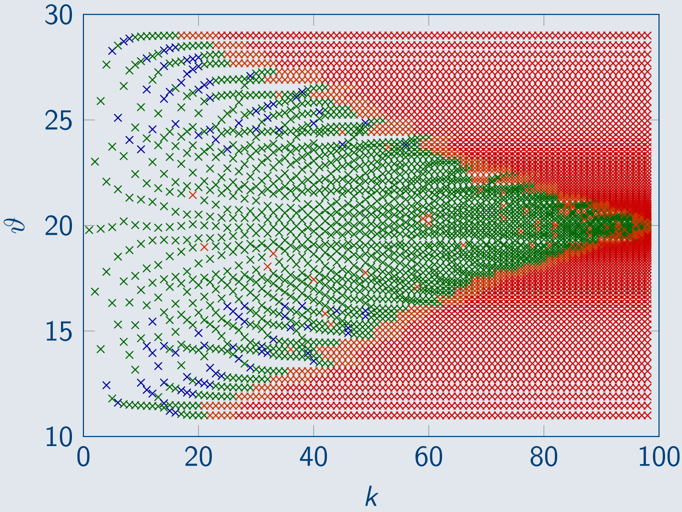

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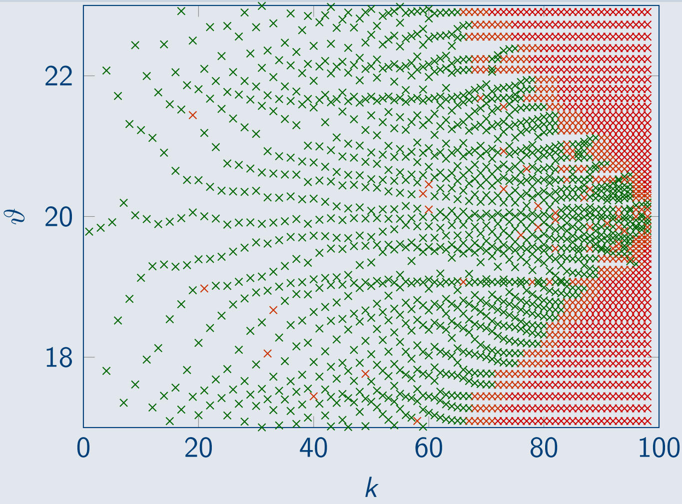

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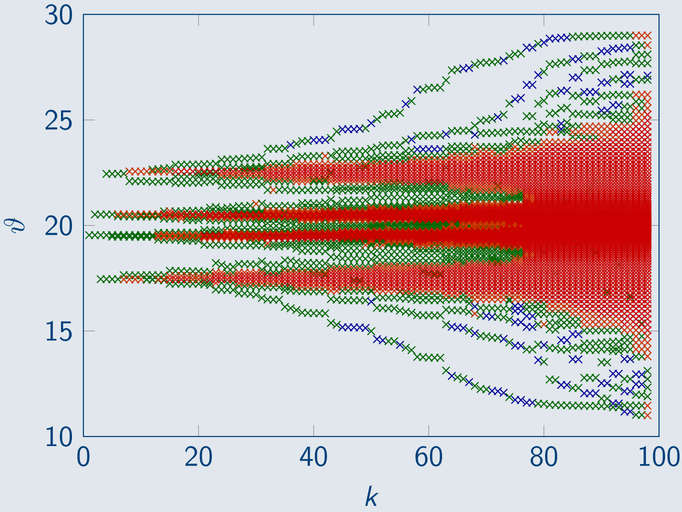

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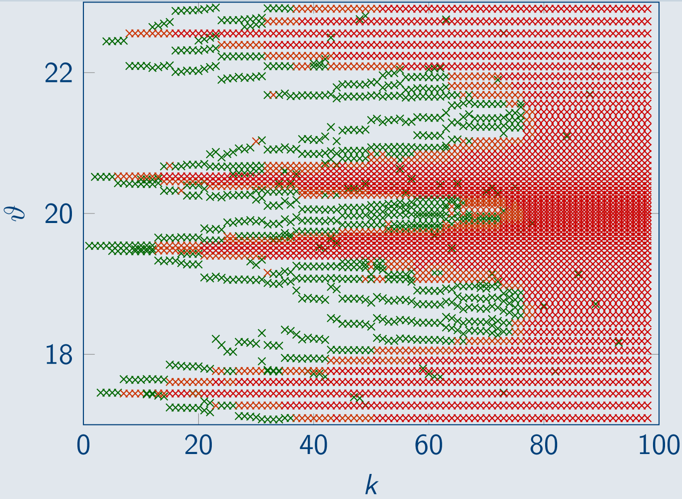

Rational Krylov methods for the GEP

Rational Arnoldi's method (Ruhe, 1998)

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

Rational Krylov methods for the GEP

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Rational Krylov

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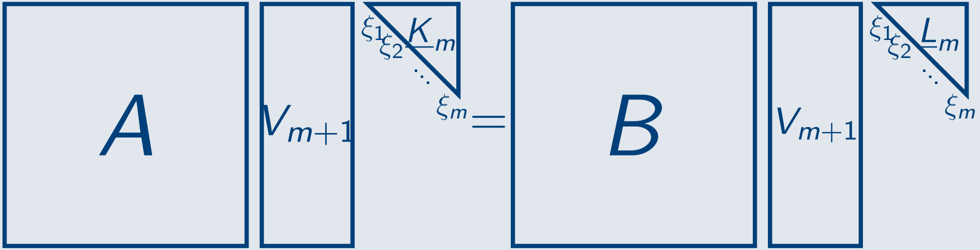

*(Abuse of) notation: ${}^{l_{i+1,i}}/_{k_{i+1,i}} = \xi_i$

Rational Krylov methods for the GEP

How to extract eigenpairs from $\mathcal{Q}_{m+1}$?

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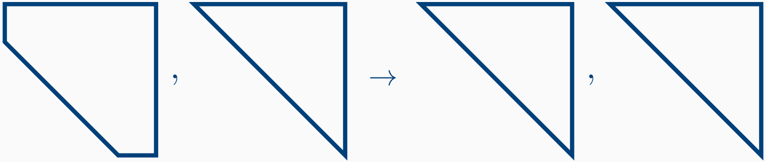
No immediate link between iterative and direct methods

(L_m, K_m) is a pair of upper Hessenberg matrices $\Rightarrow$ Moler & Stewart's implicitly shifted QZ algorithm <u>cannot</u> directly be applied.

Implicitly shifted QZ (Moler and Stewart, 1973)

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



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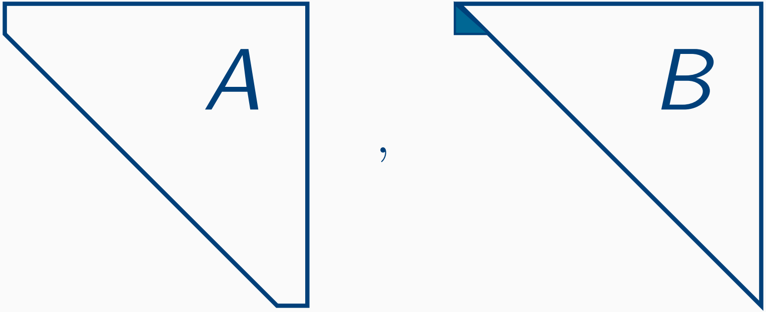

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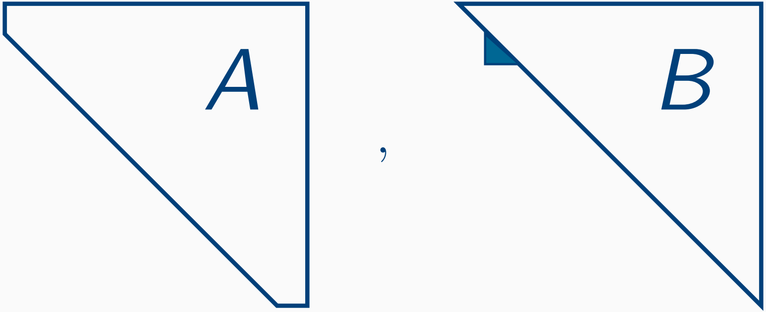

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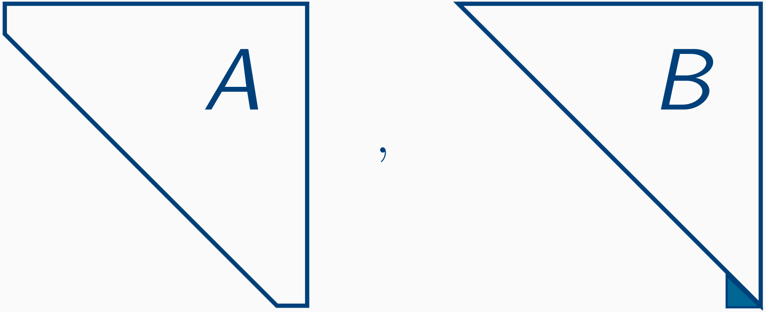

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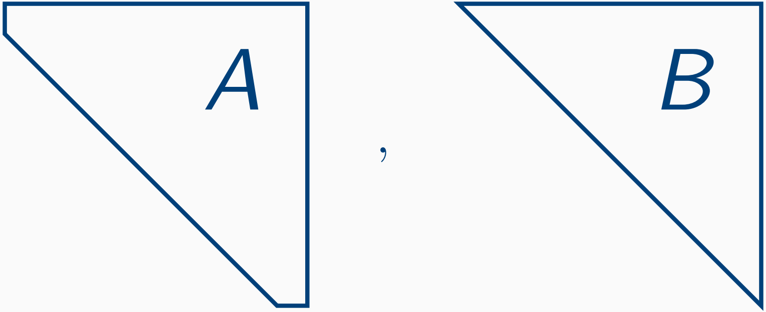

Implicitly shifted QZ (Moler and Stewart, 1973)

$$\dots$$

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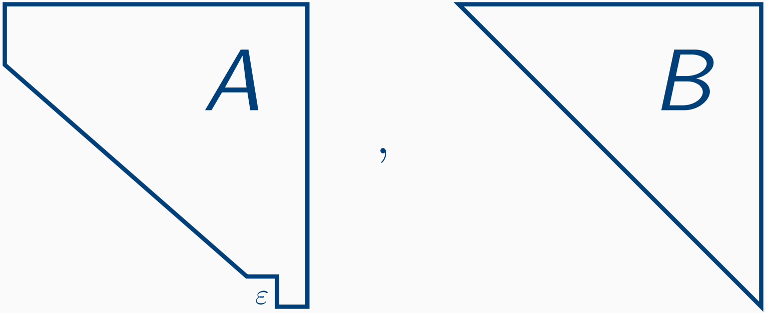
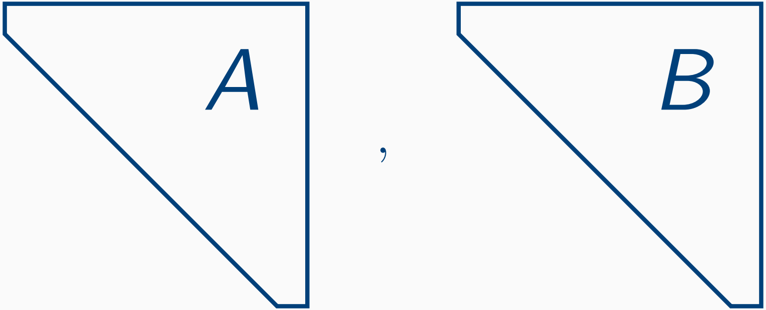
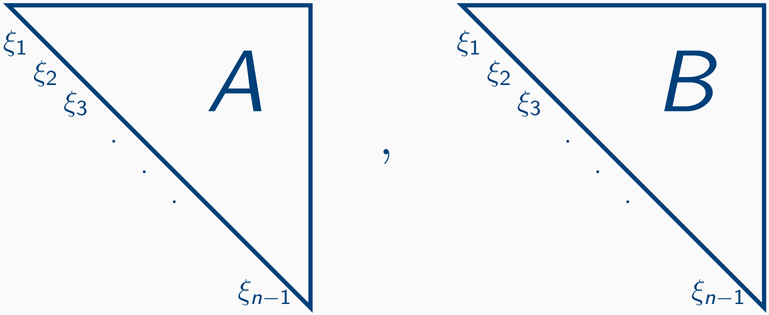


A rational QZ algorithm

Rational QZ



Rational QZ



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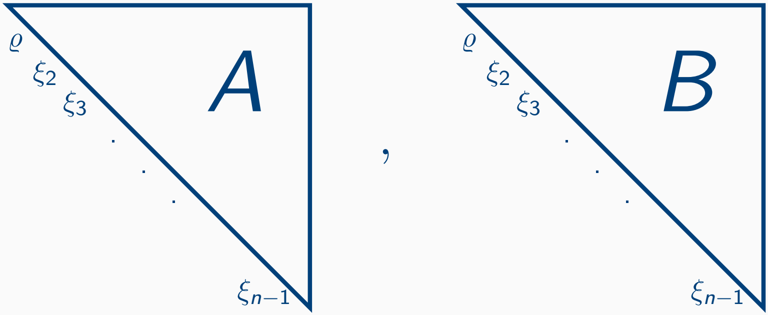

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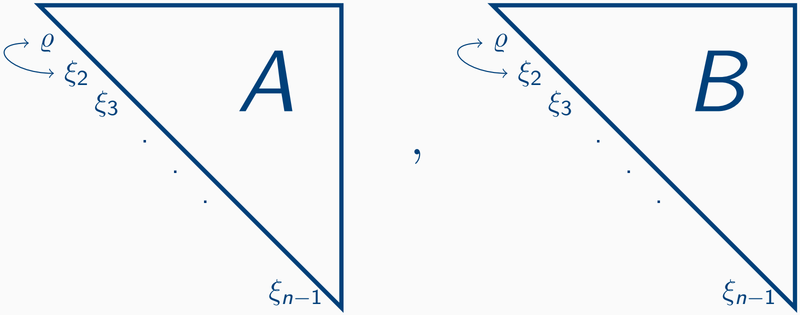

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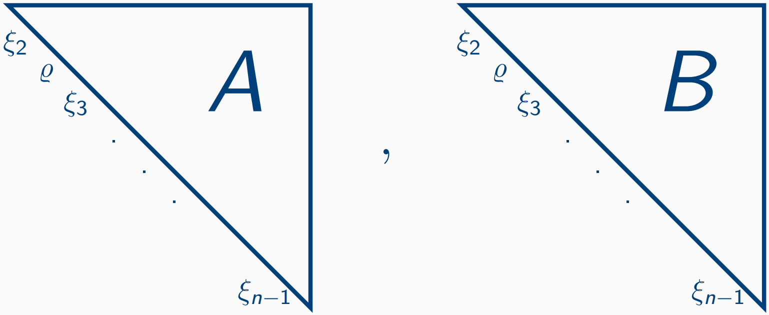

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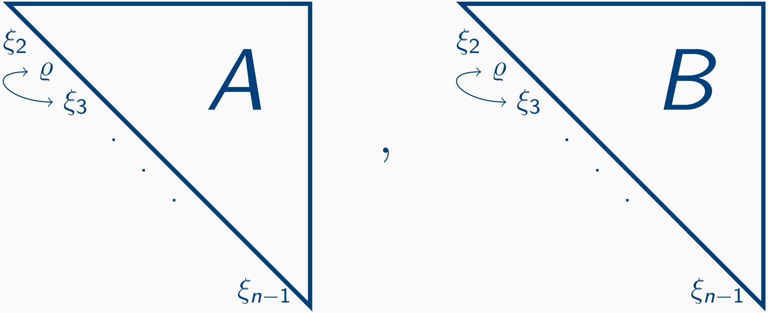
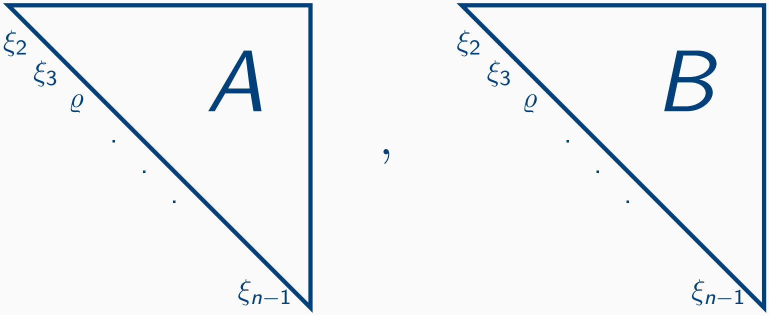


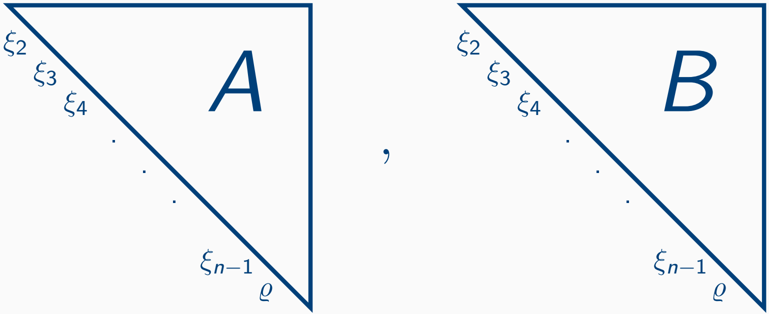
Rational QZ



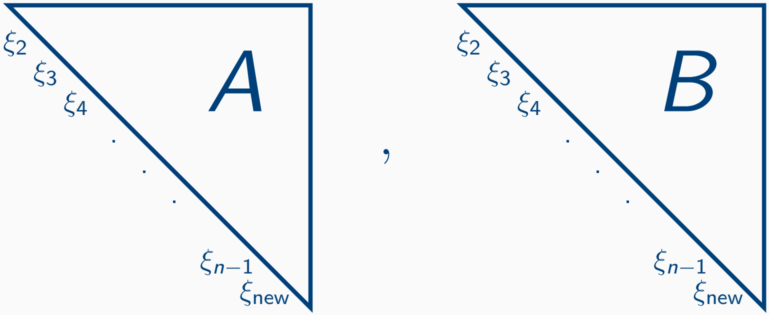
Rational QZ

$\cdots$

Rational QZ

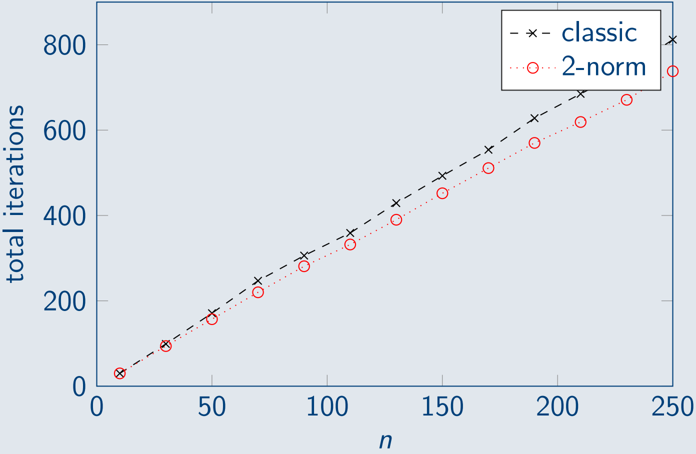


Rational QZ



Using the additional degrees of freedom — **Example 1**

Choose ξ_{new} as the rotation that minimizes the 2-norm of the vector $[a_{n-1,n}\ b_{n-1,n}]$:



Using the additional degrees of freedom **Example 1**

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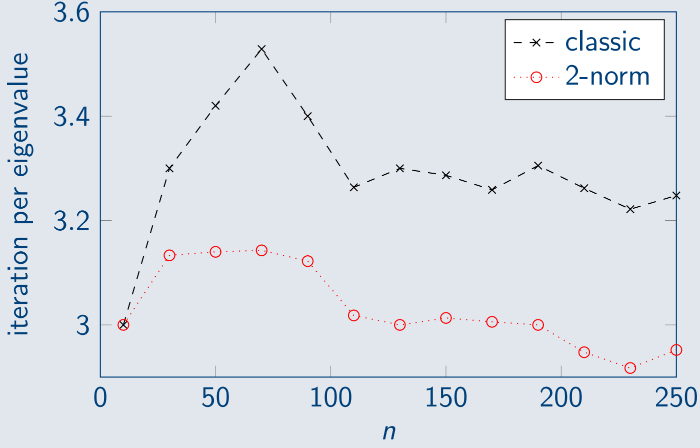
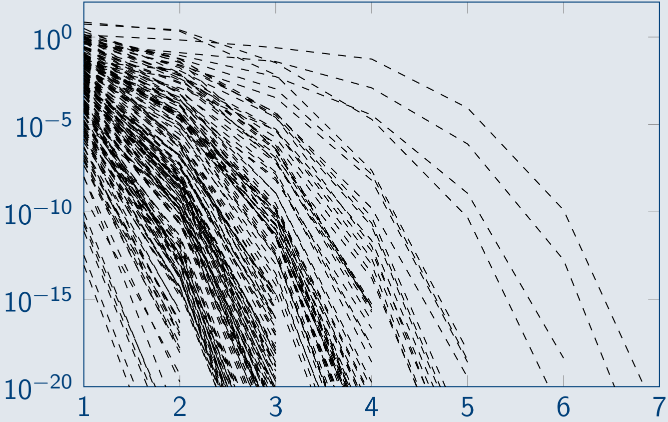


Rational QZ

Using the additional degrees of freedom **Example 1**

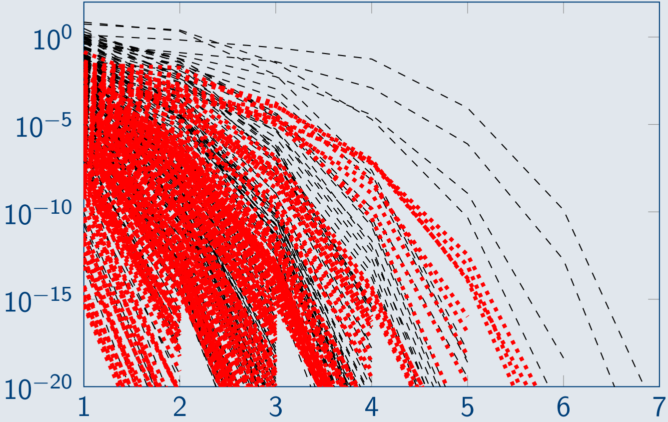
Choose ξ_{new} as the rotation that minimizes the 2-norm of the vector $[a_{n-1,n}\ b_{n-1,n}]$:



Rational QZ

Using the additional degrees of freedom **Example 1**

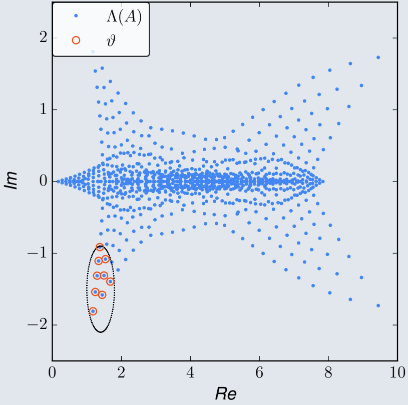
Choose ξ_{new} as the rotation that minimizes the 2-norm of the vector $[a_{n-1,n}\ b_{n-1,n}]$:



Rational QZ

Using the additional degrees of freedom **Example 2**

Choose the poles on a contour in $\mathbb{C} \rightarrow$ deflating subspaces:



Conclusion

Conclusion and outlook

Conclusion:

Polynomial Krylov	Rational Krylov
$\updownarrow$	$\updownarrow$
Francis' QR algorithm	Rational QZ algorithm

Outlook:

- Implicit steps of higher degree
- AED
- LAPACK-style software

Thank you

References

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