

Rational matrix algorithms for the generalized eigenvalue problem

Iterative and direct methods

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Overview

Part I

Standard eigenvalue problem

Large scale: Polynomial Krylov



Medium scale: Francis' QR algorithm

Part II

Generalized eigenvalue problem

Large scale: Rational Krylov



Medium scale: Rational QZ algorithm

Part I: Polynomial methods

Standard eigenvalue problem (SEP)

Definition SEP

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

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

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

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10^6	32 years

Polynomial Krylov methods for the SEP

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

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

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

Then

$$\exists p \in \mathcal{P}_\ell : p(A)\mathbf{v} = a_0\mathbf{v} + a_1A\mathbf{v} + \dots + a_\ell A^\ell\mathbf{v} = \mathbf{0} \quad \text{with } a_\ell \neq 0$$

Polynomial Krylov methods for the SEP

If we factorize:

$$p(A)\mathbf{v} = \prod_{i=1}^{\ell} (A - \lambda_i I) \mathbf{v} = \mathbf{0}$$

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Definition polynomial Krylov subspace

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

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

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- $m = \ell$:
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 - \mathcal{K}_{m+1} often *contains* accurate approximations to some eigenpairs of A .

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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 x_1 . Then

$$\|A^k v - x_1\| = \mathcal{O}\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$$

⇒ this rapidly becomes a very ill-conditioned basis!

Polynomial Krylov methods for the SEP (Arnoldi, 1951)

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

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$$\begin{array}{c|c|c} m = 0 & \mathcal{K}_1 & \mathbf{v}_1 = \mathbf{v}/\|\mathbf{v}\| \\ \hline m = 1 & \mathcal{K}_2 & \mathbf{v}_1 \\ & & h_{11} = \mathbf{v}_1^* A \mathbf{v}_1 & h_{21} \mathbf{v}_2 = A \mathbf{v}_1 - h_{11} \mathbf{v}_1 \end{array}$$

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$m = 0$	\mathcal{K}_1	$\mathbf{v}_1 = \mathbf{v}/\ \mathbf{v}\ $		
$m = 1$	\mathcal{K}_2	\mathbf{v}_1	$h_{11} = \mathbf{v}_1^* A \mathbf{v}_1$	$h_{21} \mathbf{v}_2 = A \mathbf{v}_1 - h_{11} \mathbf{v}_1$
\vdots	\vdots	\vdots	\vdots	\vdots
$m = k$	\mathcal{K}_{k+1}	$\mathbf{v}_1 \dots \mathbf{v}_k$	$h_{1k} = \mathbf{v}_1^* A \mathbf{v}_k$	$h_{k+1,k} \mathbf{v}_{k+1} = A \mathbf{v}_k - h_{1k} \mathbf{v}_1 - \dots - h_{kk} \mathbf{v}_k$ (\star)
			\vdots	
			$h_{kk} = \mathbf{v}_k^* A \mathbf{v}_k$	

Polynomial Krylov methods for the SEP (Arnoldi, 1951)

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

At step k :

$$A\mathbf{v}_k = h_{1k}\mathbf{v}_1 + \dots + h_{kk}\mathbf{v}_k + h_{k+1,k}\mathbf{v}_{k+1} \quad (\star)$$

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

At step k :

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

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

Combining all m steps:

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

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Combining all m steps:

$$A \quad V_m = V_{m+1} \quad H_m$$

The diagram illustrates the Arnoldi iteration process. It shows a large square matrix A on the left, followed by an equals sign. To the right of the equals sign is another large square matrix V_m , which is followed by a right-pointing arrow and a larger square matrix V_{m+1} . To the right of V_{m+1} is a smaller square matrix labeled H_m , which is tilted at approximately a 45-degree angle.

Column k satisfies Eq. (★)

Polynomial Krylov methods for the SEP

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

⇒ Compute the **Ritz pairs**:

$$H_m \mathbf{z} = \vartheta \mathbf{z}$$

Ritz pairs $(\vartheta, \mathbf{x}) := (\vartheta, V_m \mathbf{z})$

Polynomial Krylov methods for the SEP

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Link between iterative and direct methods

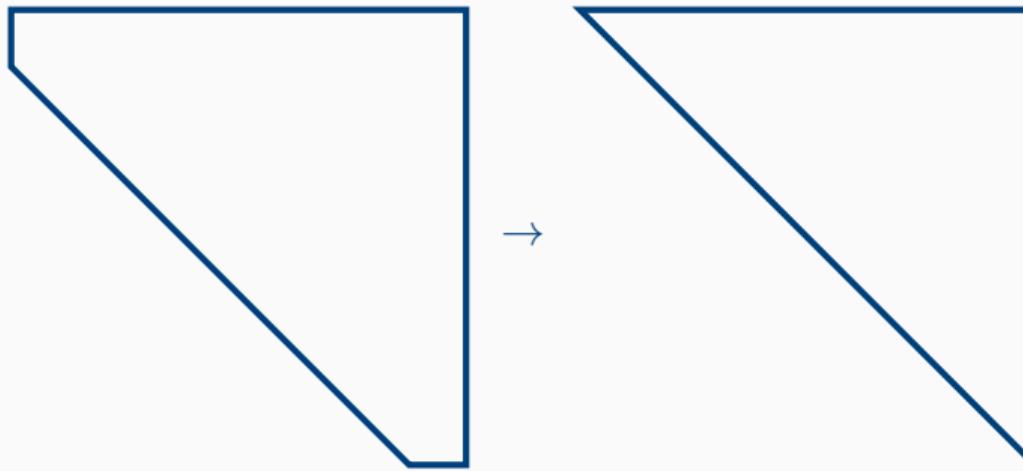
H_m upper Hessenberg matrix ⇒ Francis' implicitly shifted QR

Implicitly shifted QR (Francis, 1961, 1962)

A

\rightarrow

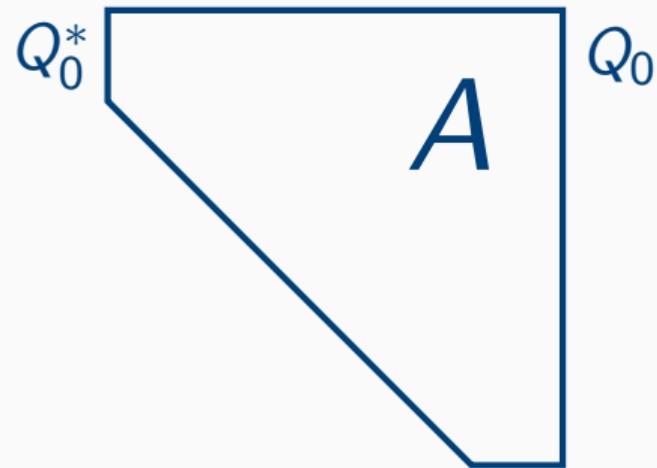
$\hat{A} = Q^* A Q$



Implicitly shifted QR (Francis, 1961, 1962)

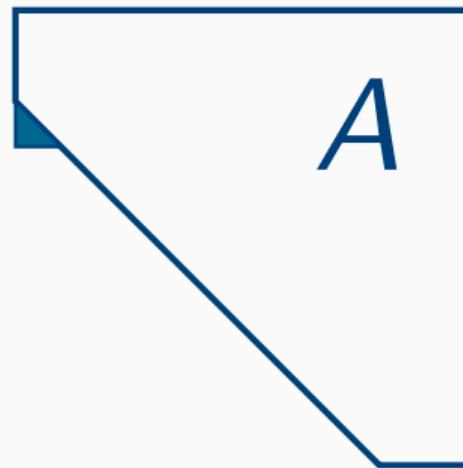


Implicitly shifted QR (Francis, 1961, 1962)

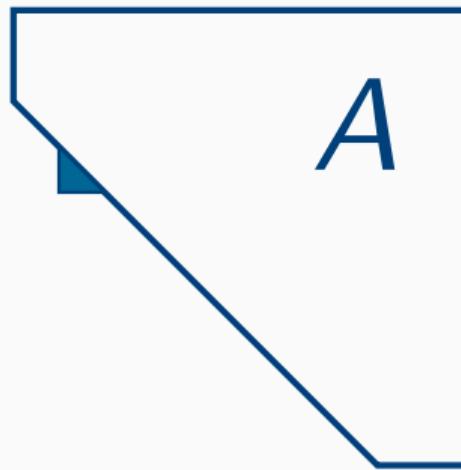


$$Q_0 \mathbf{e}_1 = \alpha(A - \varrho I)\mathbf{e}_1$$

Implicitly shifted QR (Francis, 1961, 1962)



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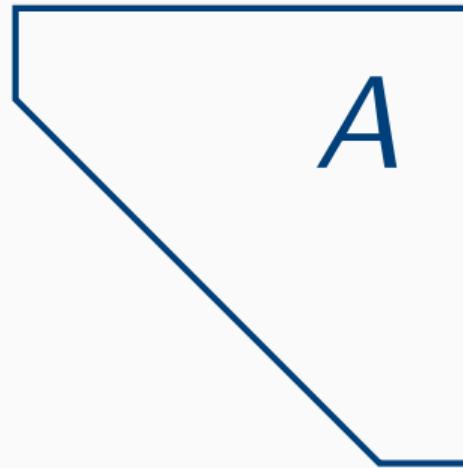
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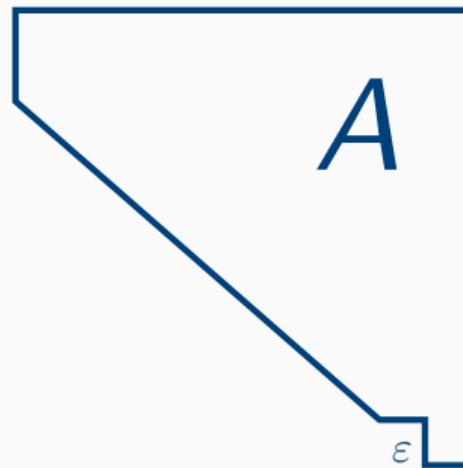
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Part II: Rational methods

Generalized eigenvalue problem (GEP)

Definition GEP

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

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

Rational Krylov methods for the GEP

$$A : \quad \mathcal{K}_{m+1} \mid \mathbf{v}, A\mathbf{v}, \dots, A^m\mathbf{v}$$

Rational Krylov methods for the GEP

$$\begin{array}{ll} A : & \mathcal{K}_{m+1} \left| \begin{array}{l} \mathbf{v}, A\mathbf{v}, \dots, A^m\mathbf{v} \end{array} \right. \\ (A, B) : & \mathcal{K}_{m+1} \left| \begin{array}{l} \mathbf{v}, B^{-1}A\mathbf{v}, \dots, (B^{-1}A)^m\mathbf{v} \end{array} \right. \end{array}$$

Rational Krylov methods for the GEP

$$\begin{array}{ll} A : & \mathcal{K}_{m+1} \mid \mathbf{v}, A\mathbf{v}, \dots, A^m\mathbf{v} \\ (A, B) : & \mathcal{K}_{m+1} \mid \mathbf{v}, B^{-1}A\mathbf{v}, \dots, (B^{-1}A)^m\mathbf{v} \\ (A, B) : & \mathcal{Q}_{m+1} \mid \mathbf{v}, M_1\mathbf{v}, \dots, M_m\mathbf{w} \end{array}$$

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

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

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

Rational Krylov methods for the GEP

Special choices for (♣) :

- *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 ($M = (A - \xi B)^{-1}B$)

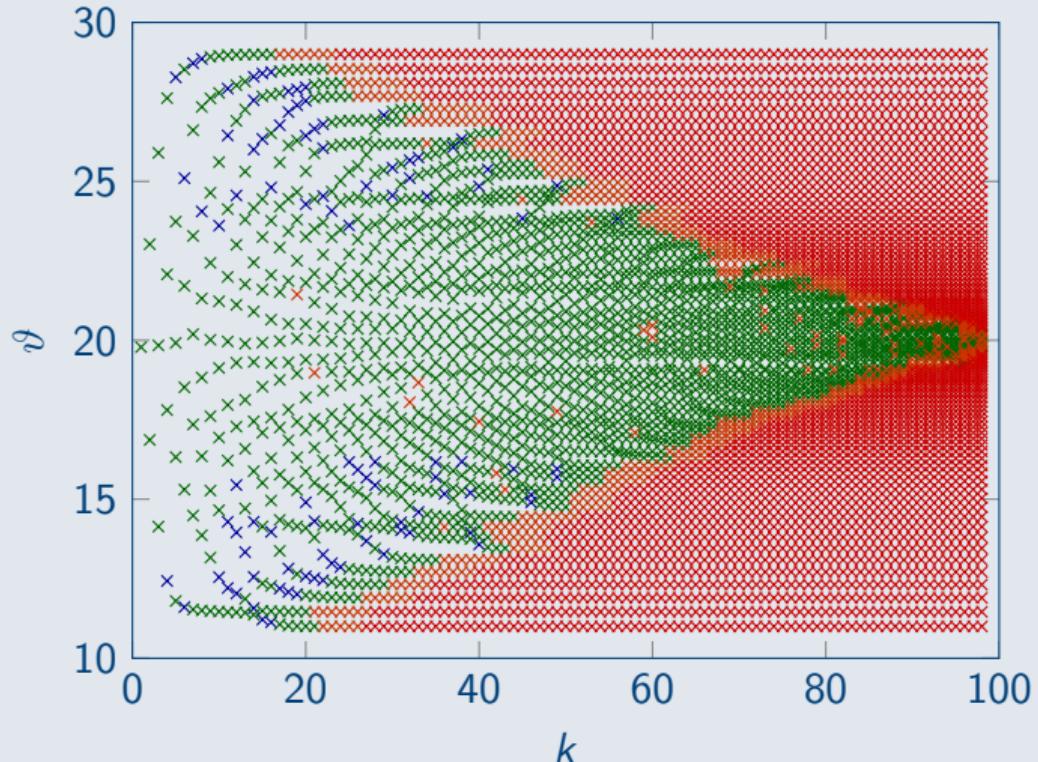
Rational Krylov methods for the GEP

Motivation for using rational methods



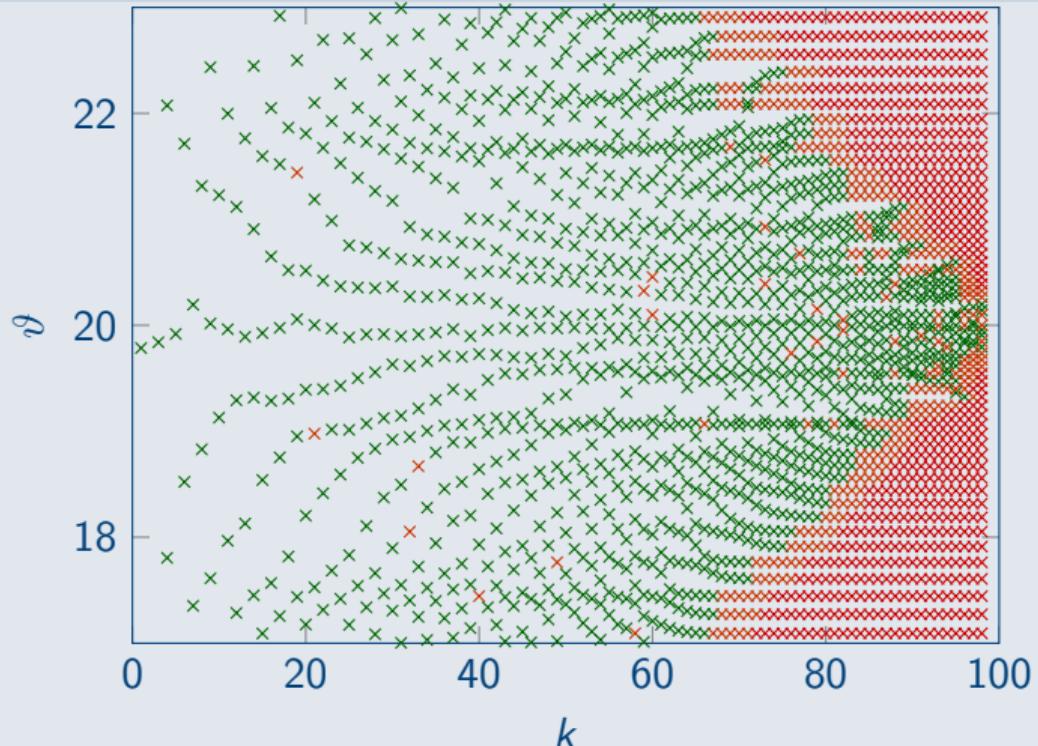
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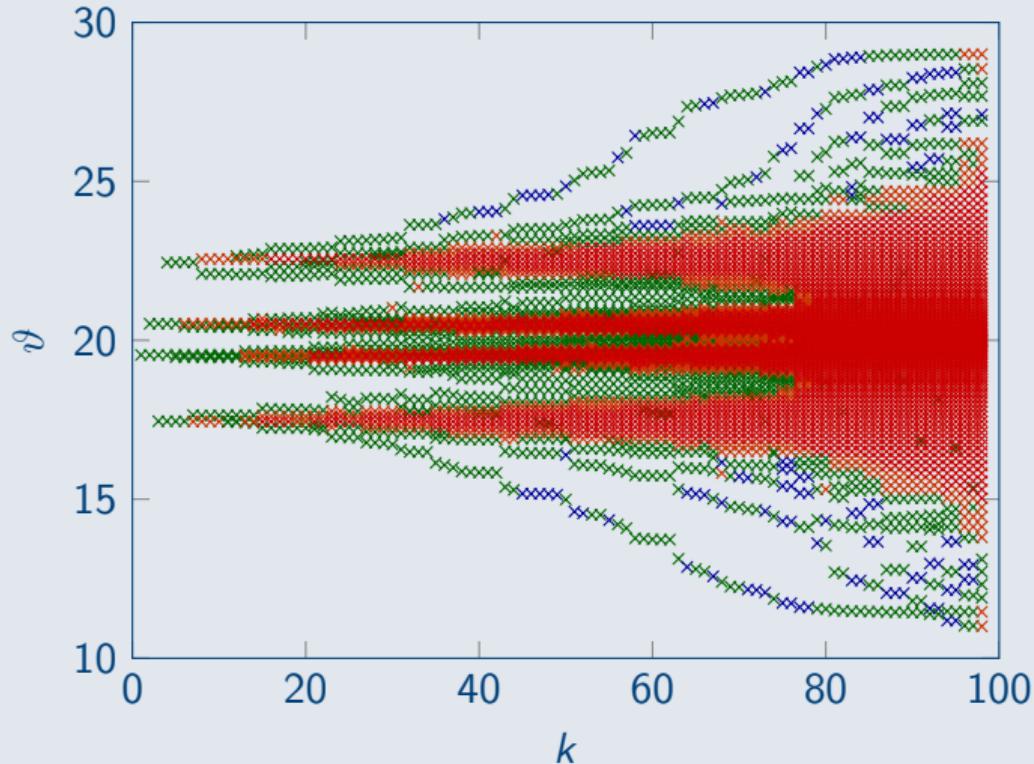
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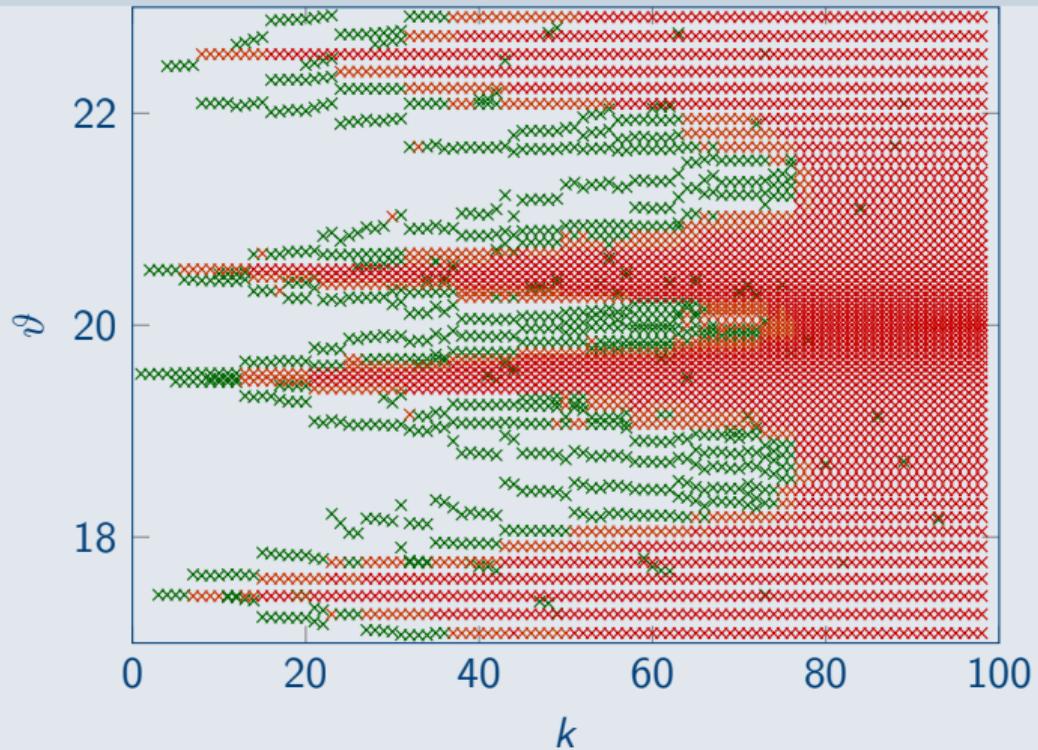
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Rational Krylov methods for the GEP

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

Rational Arnoldi's method (Ruhe, 1998)

$$A \begin{pmatrix} V_{m+1} \\ \vdots \end{pmatrix} = B \begin{pmatrix} V_{m+1} \\ \vdots \end{pmatrix} + \underline{K}_m$$

Rational Krylov

Rational Arnoldi's method (Ruhe, 1998)

$$A \begin{matrix} \\ V_{m+1} \end{matrix} \begin{matrix} \cancel{\xi_1} \\ \cancel{\xi_2} \\ \ddots \\ \cancel{\xi_m} \end{matrix} = \begin{matrix} \\ B \end{matrix} \begin{matrix} \\ V_{m+1} \end{matrix} \begin{matrix} \cancel{\xi_1} \\ \cancel{\xi_2} \\ \ddots \\ \cancel{\xi_m} \end{matrix}$$

*(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} ?

⇒ Compute the **Ritz pairs**:

$$L_m \mathbf{z} = \vartheta K_m \mathbf{z}$$

Ritz pairs $(\vartheta, \mathbf{x}) := (\vartheta, V_{m+1} K_m \mathbf{z})$

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No immediate link between iterative and direct methods

(L_m, K_m) is a pair of upper Hessenberg matrices ⇒ Moler & Stewart's implicitly shifted QZ algorithm cannot directly be applied.

Implicitly shifted QZ (Moler and Stewart, 1973)

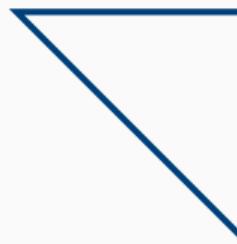
$$(A, B)$$

→

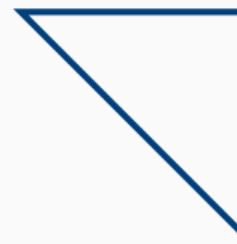
$$(\hat{A}, \hat{B}) = Q^* (A, B) Z$$



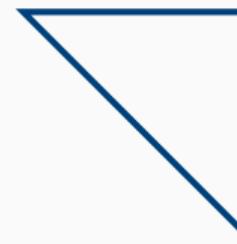
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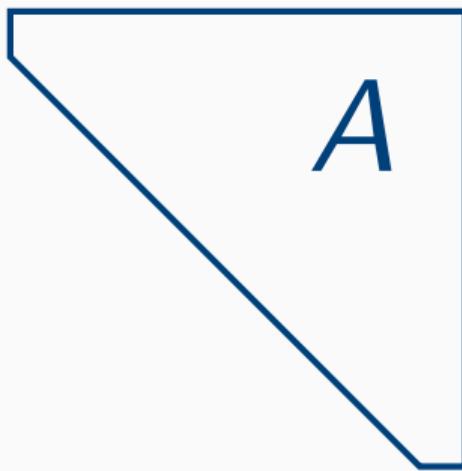
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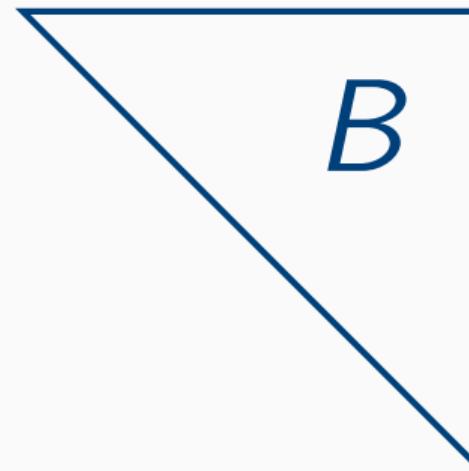
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Implicitly shifted QZ (Moler and Stewart, 1973)



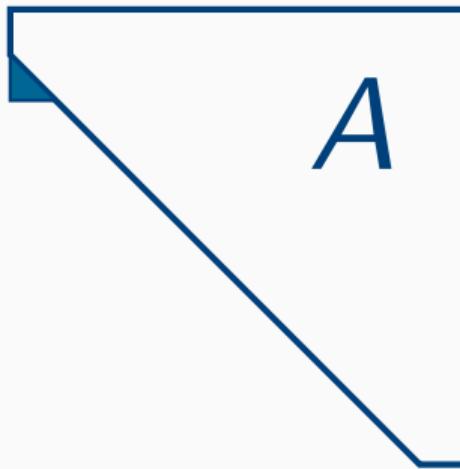
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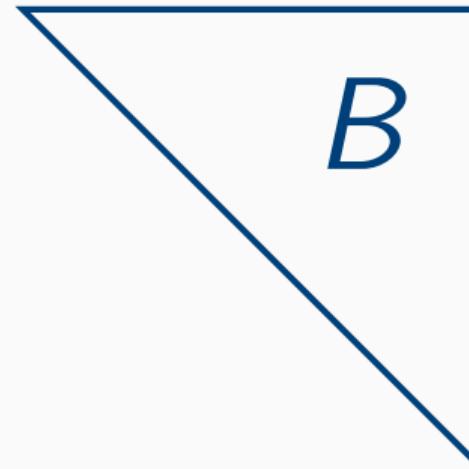
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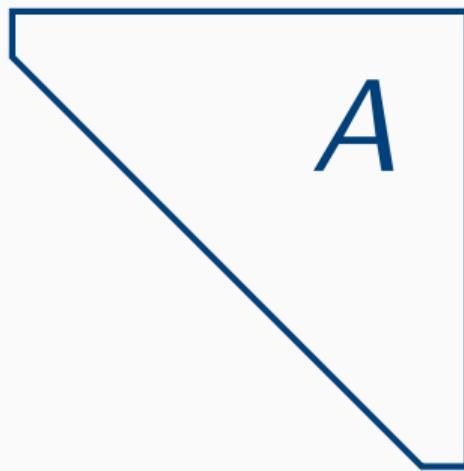
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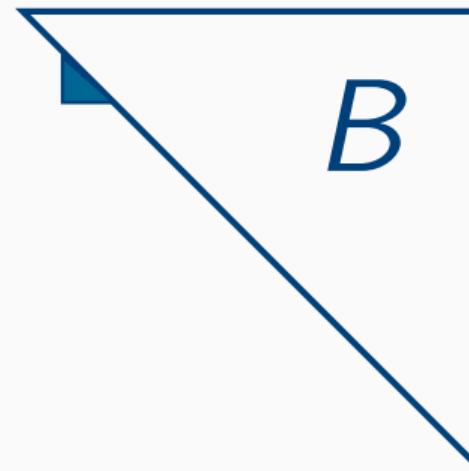
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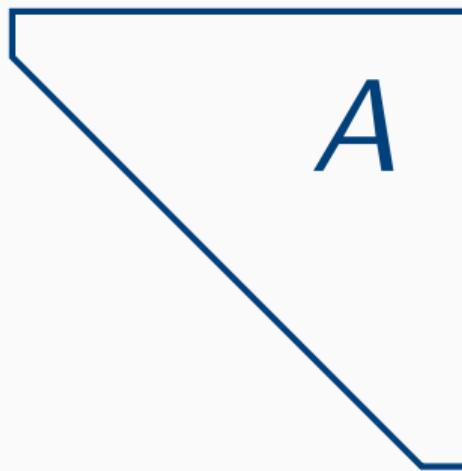
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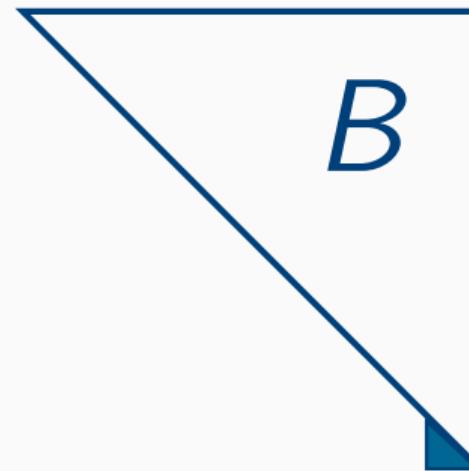
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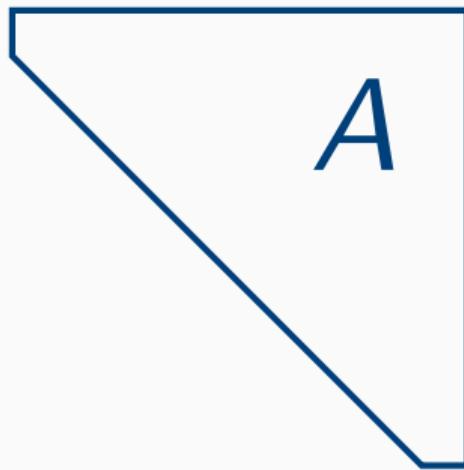
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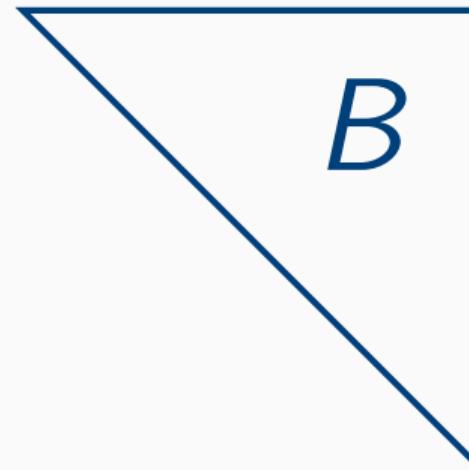
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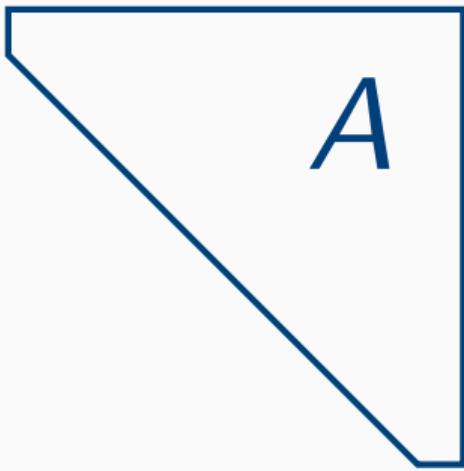
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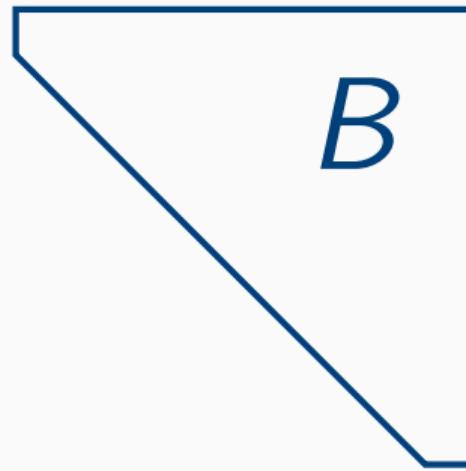


A rational QZ algorithm

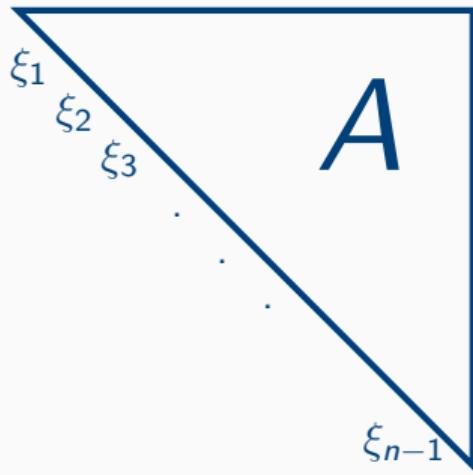
Rational QZ



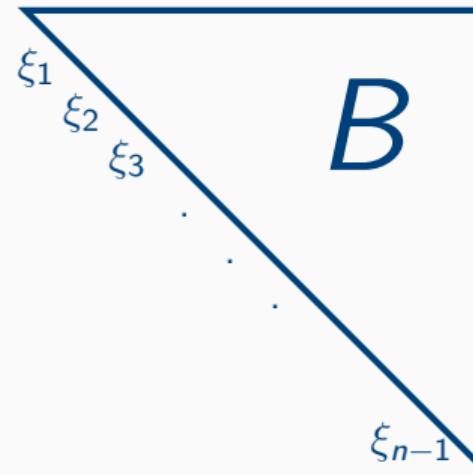
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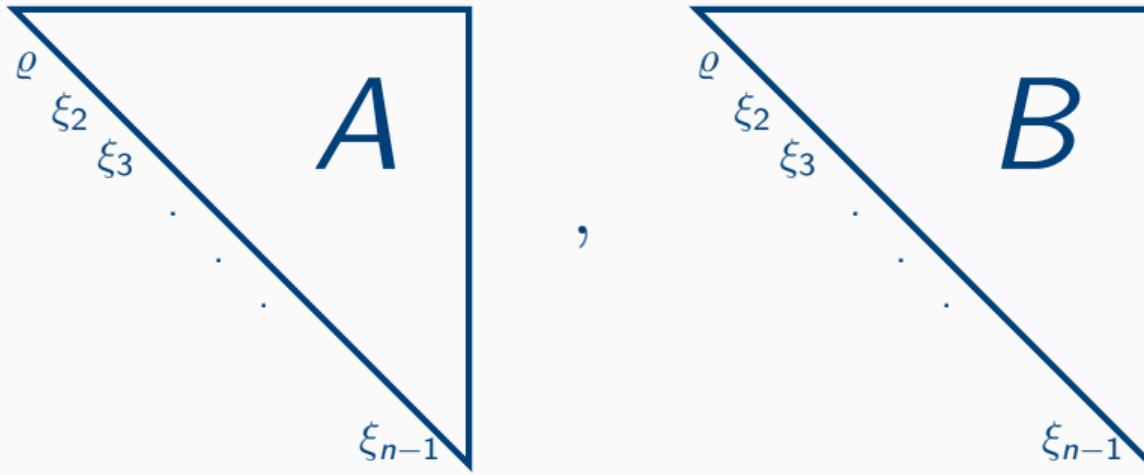
Rational QZ



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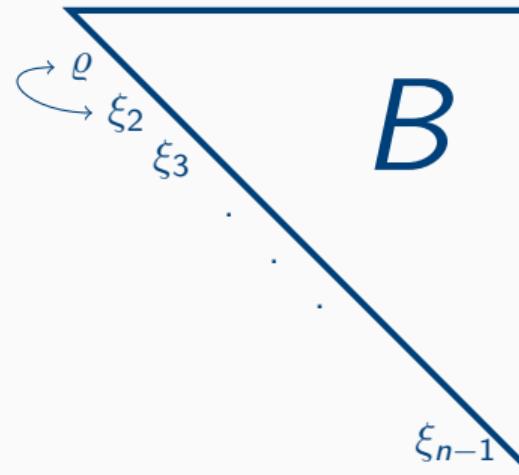
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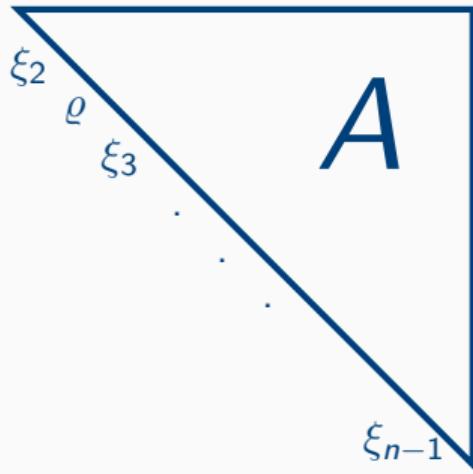
Rational QZ



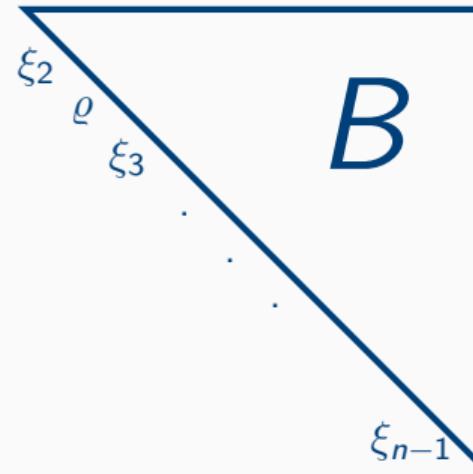
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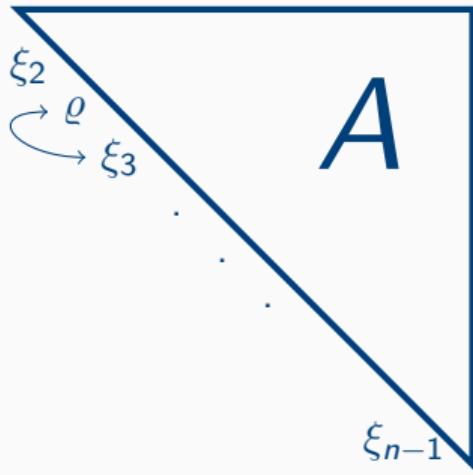
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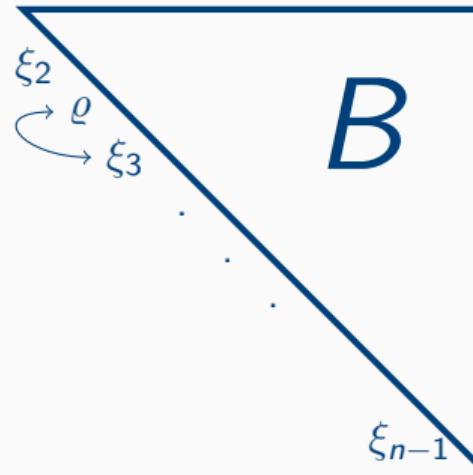
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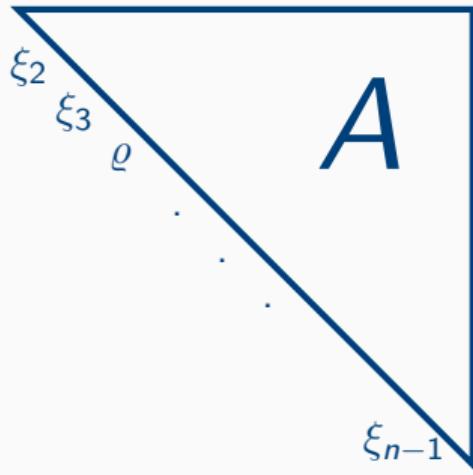
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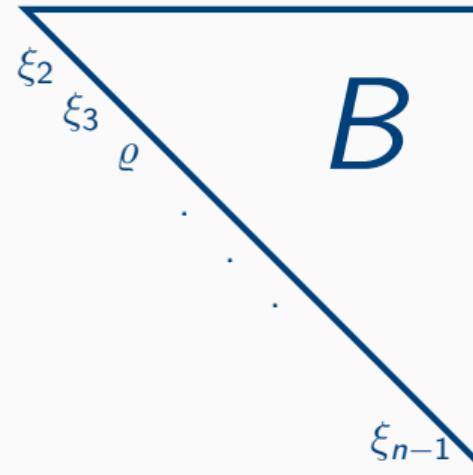
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Rational QZ



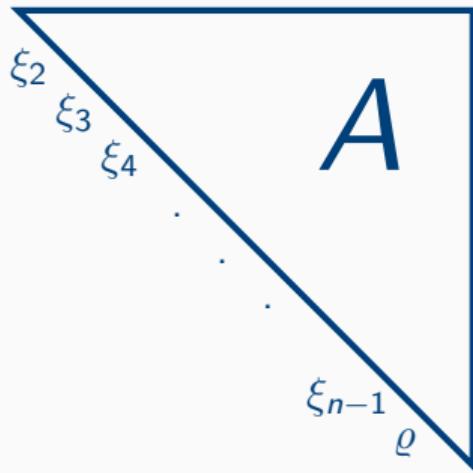
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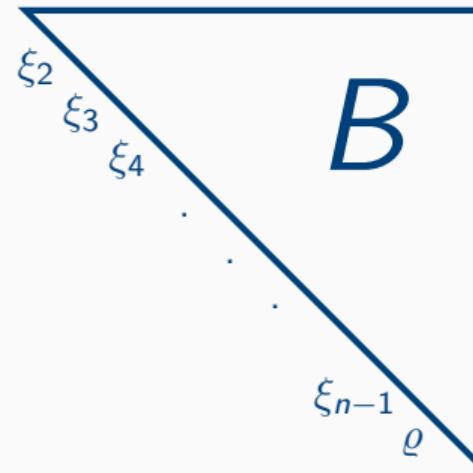
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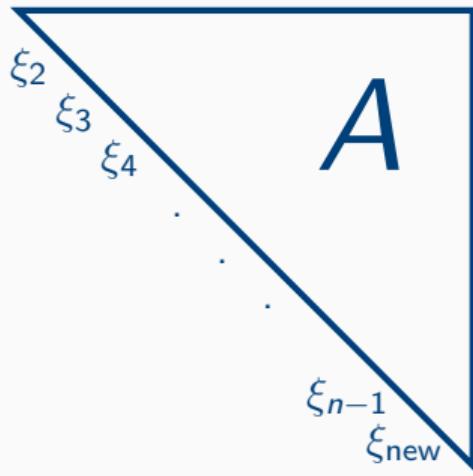
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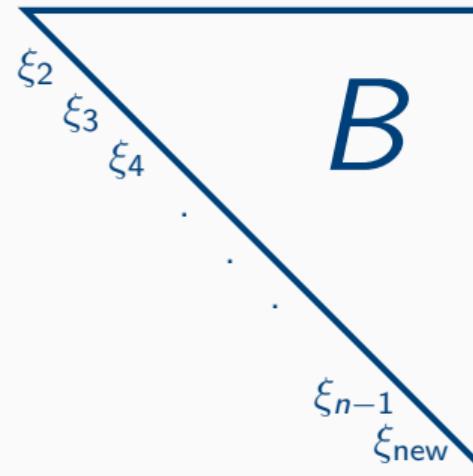
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Rational QZ



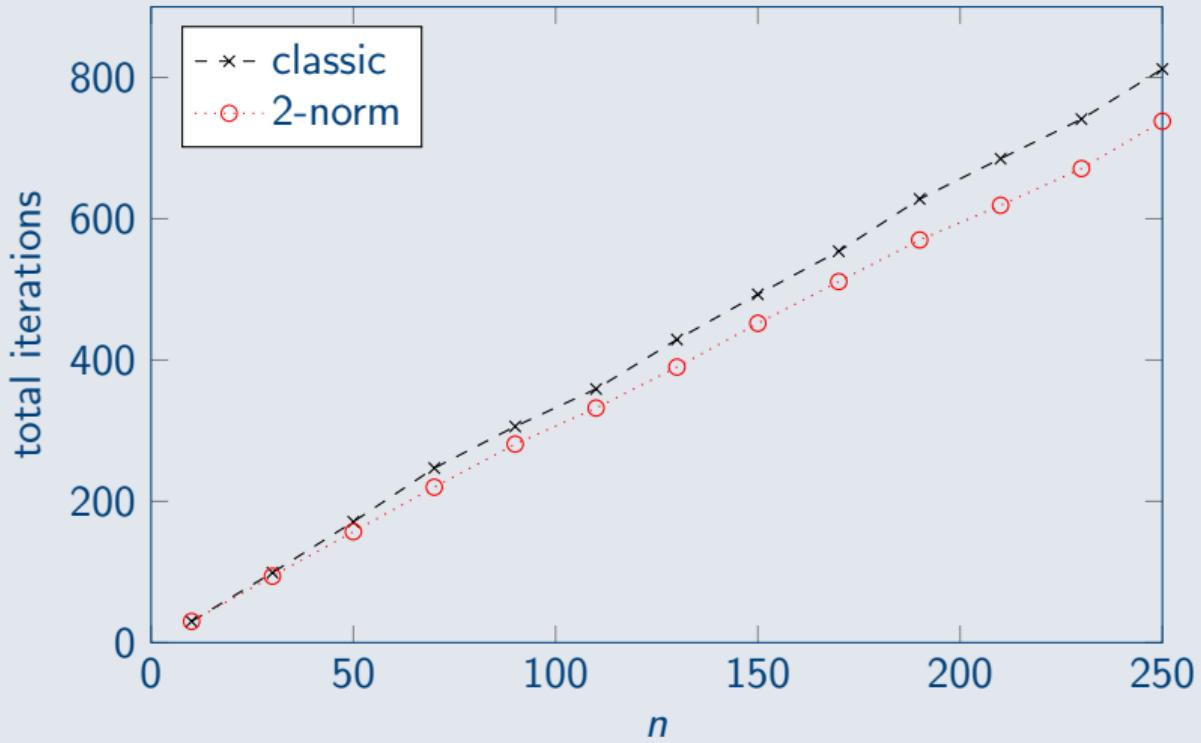
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Rational QZ

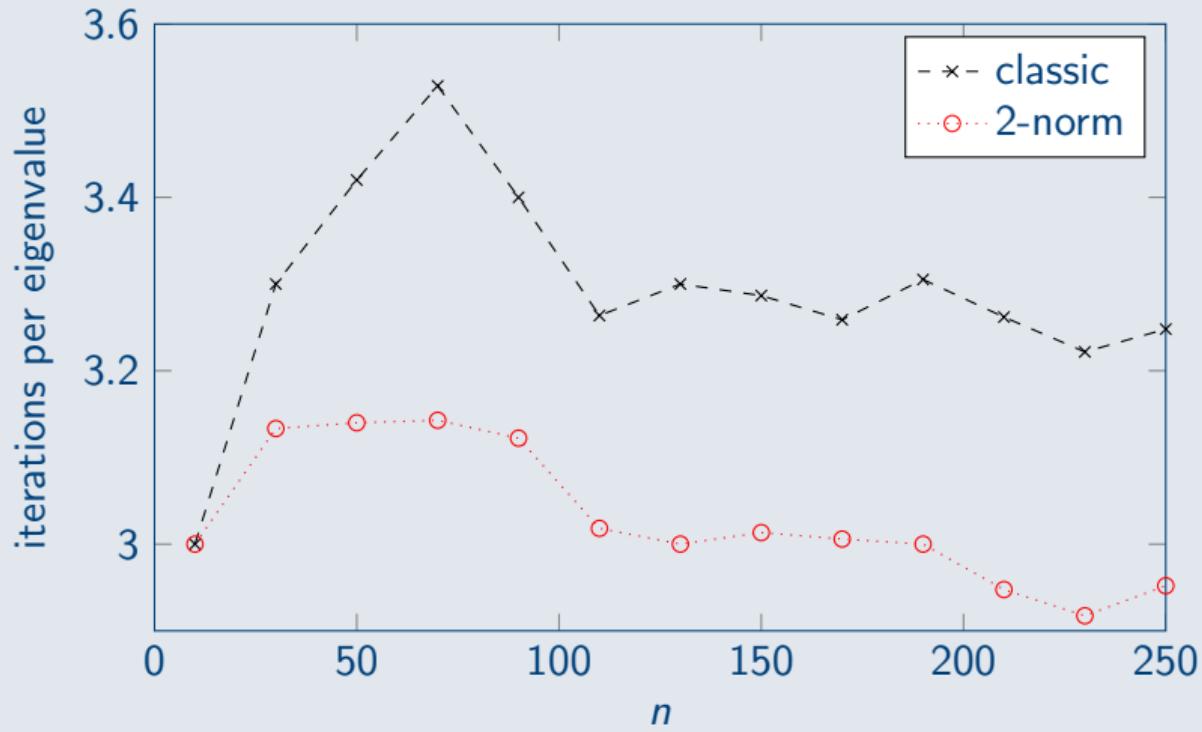
Using the additional degrees of freedom

Example 1



Using the additional degrees of freedom

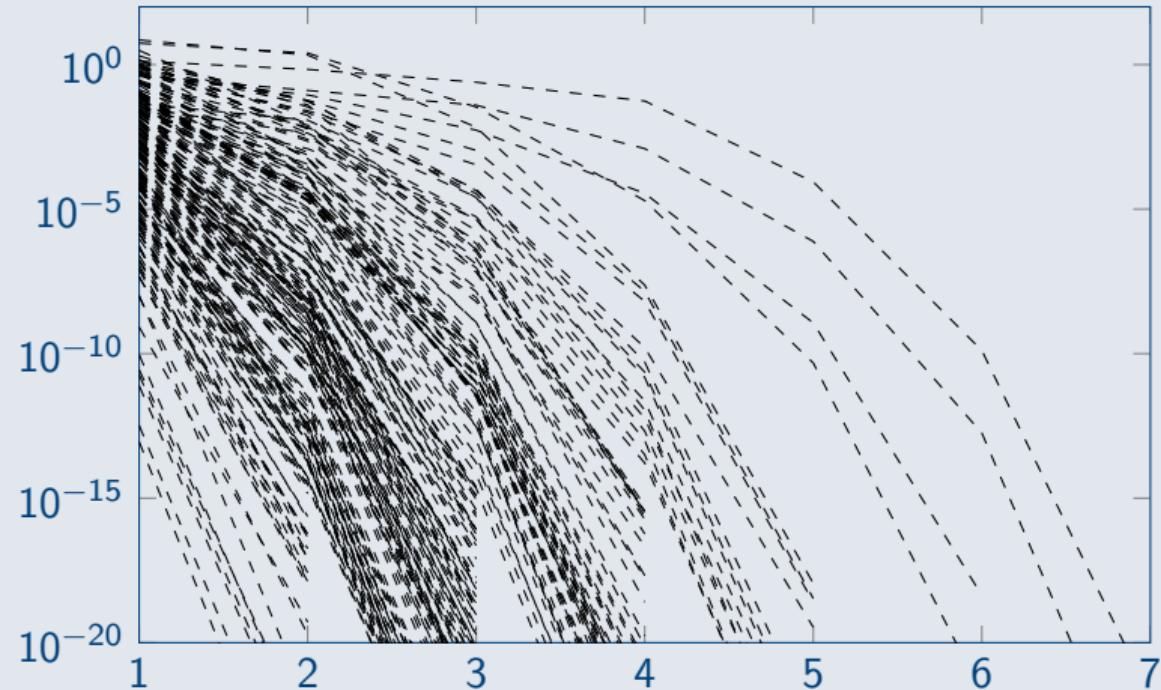
Example 1



Rational QZ

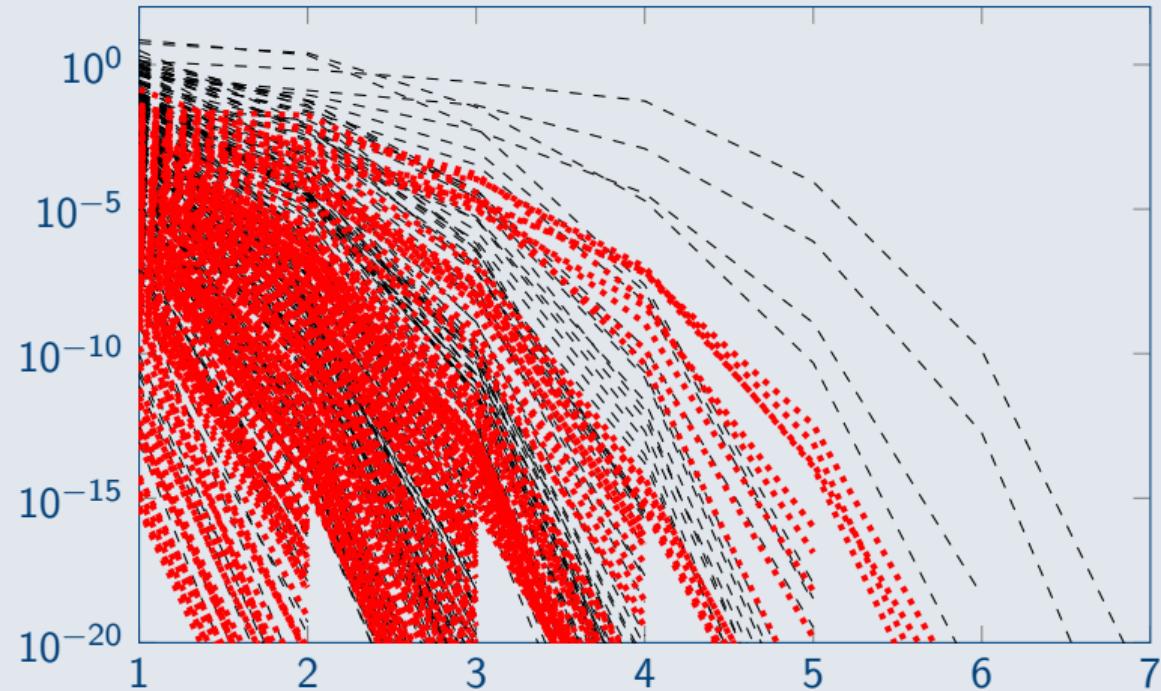
Using the additional degrees of freedom

Example 1



Using the additional degrees of freedom

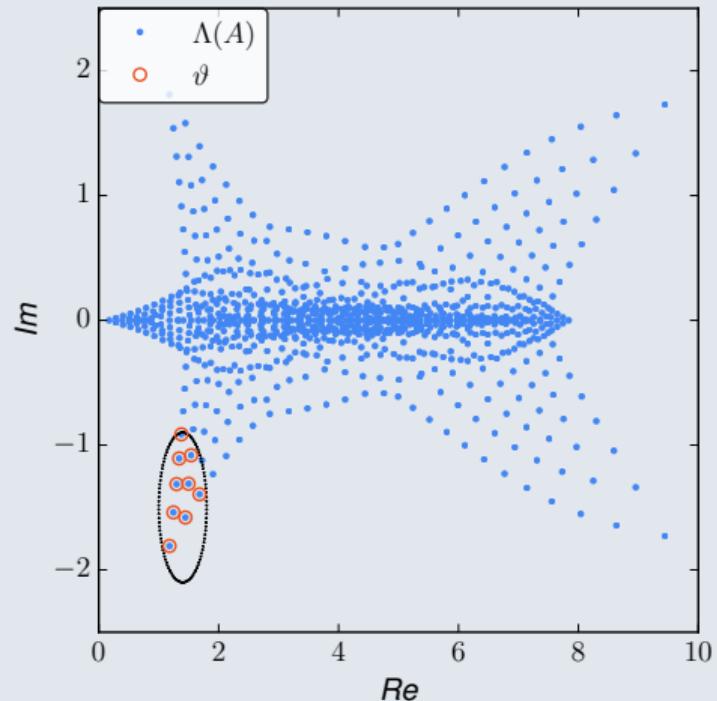
Example 1



Rational QZ

Using the additional degrees of freedom

Example 2



Conclusion

Conclusion and outlook

Conclusion:

Polynomial Krylov



Francis' QR algorithm

Rational Krylov



Rational QZ algorithm

Outlook:

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

Thank you

References

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