

# Rational matrix algorithms for the generalized eigenvalue problem

Iterative and direct methods

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# Overview

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## Part I

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Standard eigenvalue problem

*Large scale:* Polynomial Krylov



*Medium scale:* Francis' QR algorithm

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## Part II

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Generalized eigenvalue problem

*Large scale:* Rational Krylov



*Medium scale:* Rational QZ algorithm

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## Part I: Polynomial methods

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# Standard eigenvalue problem (SEP)

## Definition SEP

- $A \in \mathbb{C}^{n \times n}$
- $(\lambda, \mathbf{x})$  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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# Polynomial Krylov methods for the SEP

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

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Then

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

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If we factorize:

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

# Polynomial Krylov methods for the SEP

If we factorize:

$$p(A)\mathbf{v} = (A - \lambda_1 I) \prod_{i=2}^{\ell} (A - \lambda_i I) \mathbf{v} = (A - \lambda_1 I) \mathbf{x} = \mathbf{0}$$

⇒ we can prove that the  $\ell$  roots of  $p$  are eigenvalues of  $A$

## Definition polynomial Krylov subspace

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

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

# Polynomial Krylov methods for the SEP

- $m = \ell$ :
  - $\mathcal{K}_{m+1}$  invariant subspace of  $A$
  - $\mathcal{K}_{m+1}$  contains  $m$  eigenpairs

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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  $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_n|$  with respective eigenvectors  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ . Then

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

⇒ 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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$$m = 0 \quad \left[ \begin{array}{c} \mathcal{K}_1 \\ \vdots \end{array} \right] \quad \mathbf{v}_1 = \mathbf{v}/\|\mathbf{v}\|$$

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

# 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 ( $= 1$ )

Combining all  $m$  steps:

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

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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  $V_{m+1}$ . Further to the right is a smaller square matrix  $H_m$ , which is tilted diagonally upwards and to the right.

Column/row  $k$  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  $(\vartheta, \mathbf{x}) := (\vartheta, V_m \mathbf{z})$

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Link between iterative and direct methods

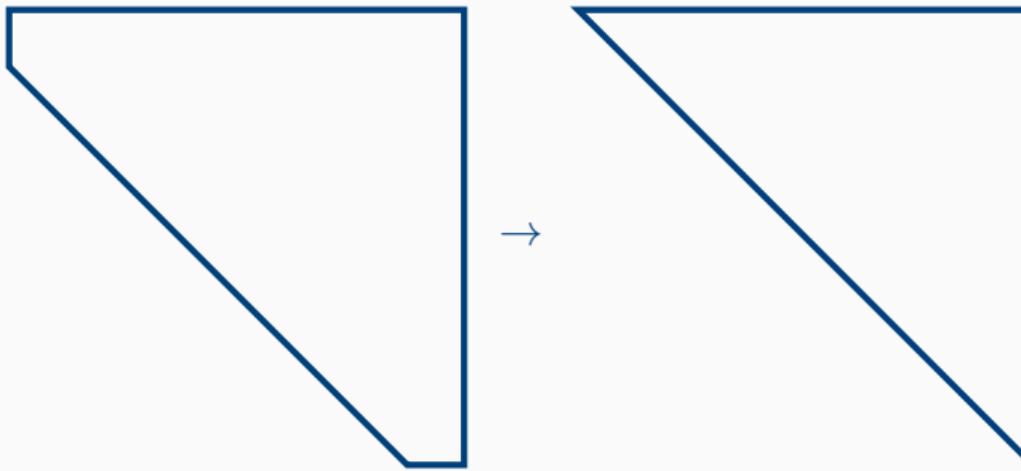
$H_m$  upper Hessenberg matrix ⇒ Francis' implicitly shifted  $QR$

## Implicitly shifted QR (Francis, 1961, 1962)

$A$

$\rightarrow$

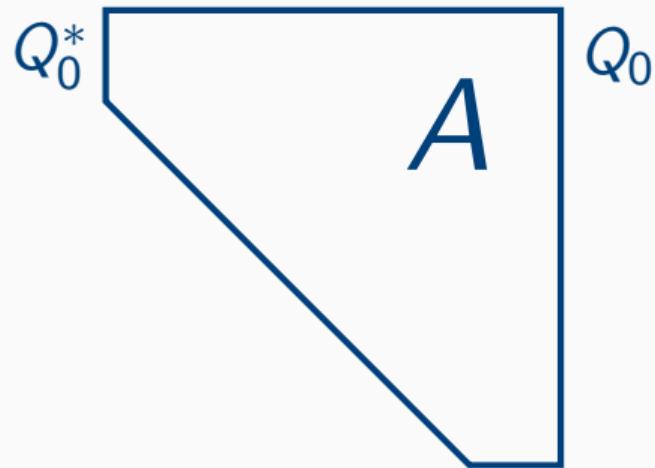
$\hat{A} = Q^* A Q$



## Implicitly shifted QR (Francis, 1961, 1962)

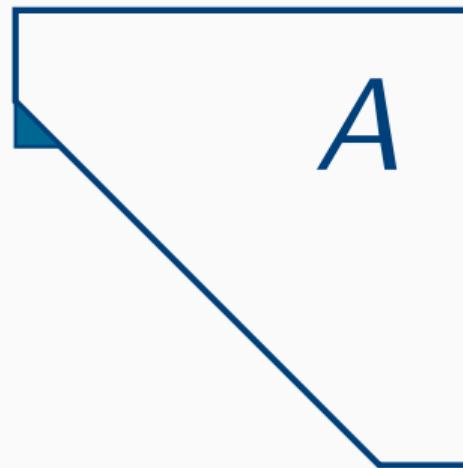


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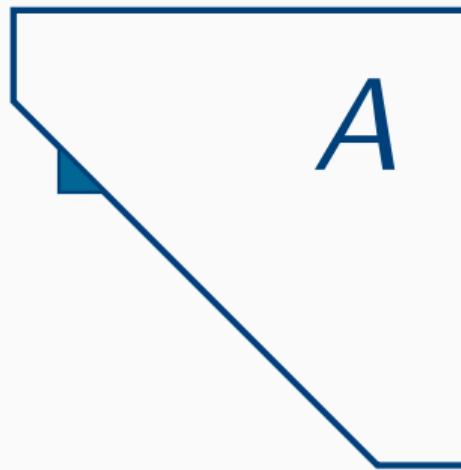


$$Q_0 \mathbf{e}_1 = \alpha(A - \varrho I)\mathbf{e}_1$$

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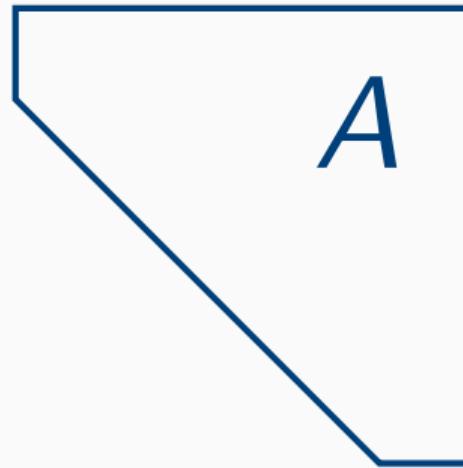
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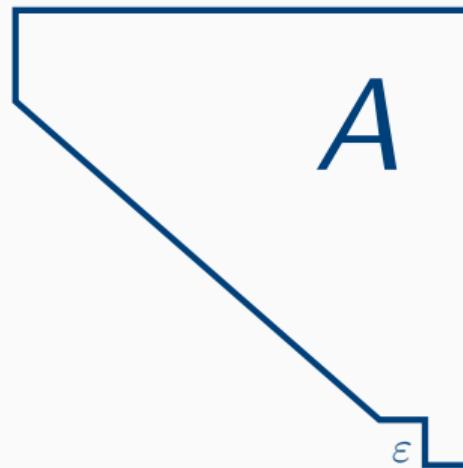
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## Part II: Rational methods

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# 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

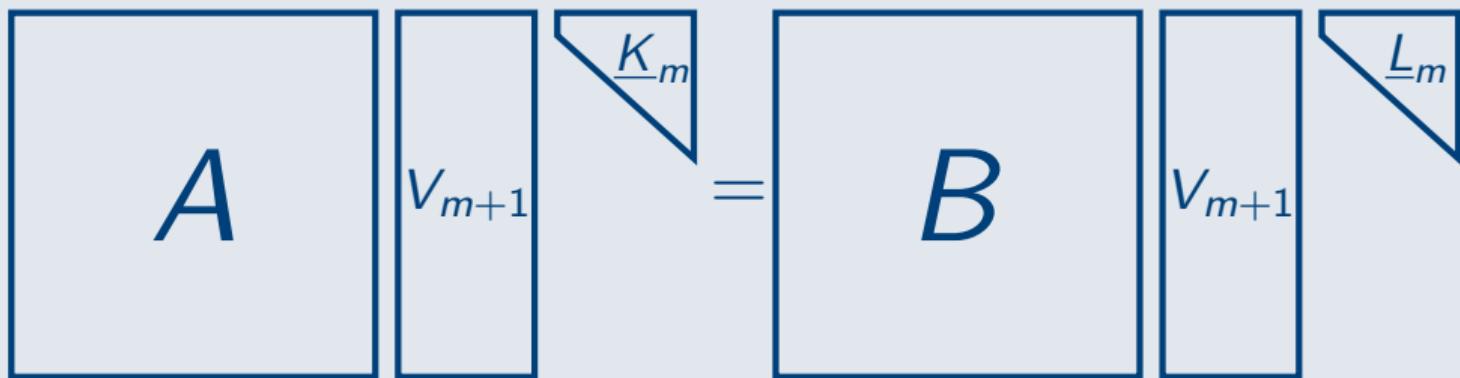
Special choices for (♣) :

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

## Rational Arnoldi's method (Ruhe, 1998)

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

## 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)

$$A \begin{matrix} \\ V_{m+1} \end{matrix} \xrightarrow[\xi_1 \quad \xi_2 \quad \ddots \quad \xi_m]{K_m} = B \begin{matrix} \\ V_{m+1} \end{matrix}$$
$$\quad \quad \quad A \begin{matrix} \\ V_{m+1} \end{matrix} \xrightarrow[\xi_1 \quad \xi_2 \quad \ddots \quad \xi_m]{L_m} = B \begin{matrix} \\ V_{m+1} \end{matrix}$$

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

# Rational Krylov

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 ⇒ Moler & Stewart's implicitly shifted QZ algorithm cannot directly be applied.

## Implicitly shifted QZ (Moler and Stewart, 1973)

$$(A, B)$$

→

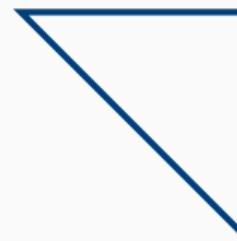
$$(\hat{A}, \hat{B}) = Q^* (A, B) Z$$



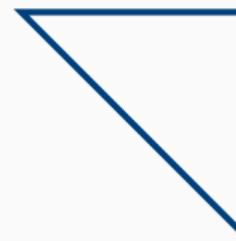
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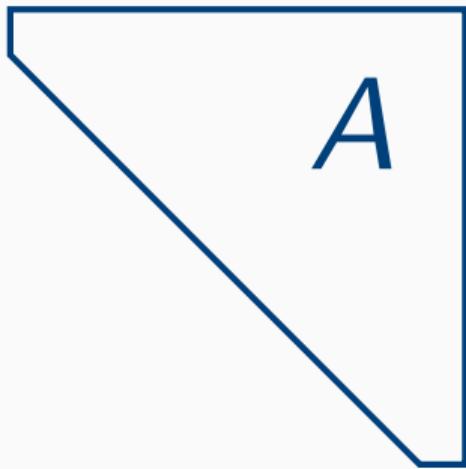
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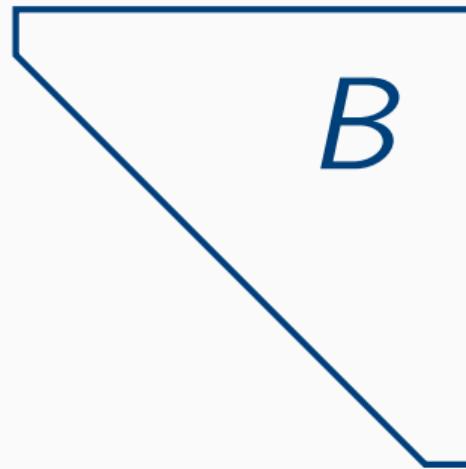
## A rational $QZ$ algorithm

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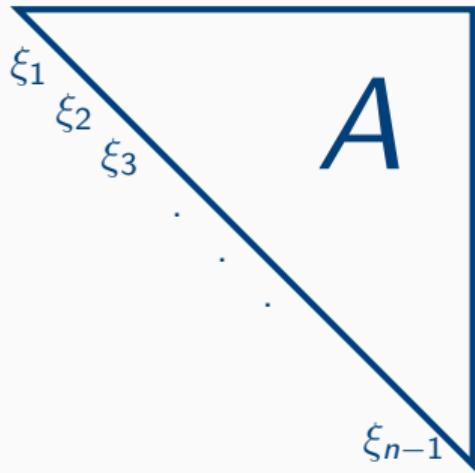
## A generalization: rational QZ



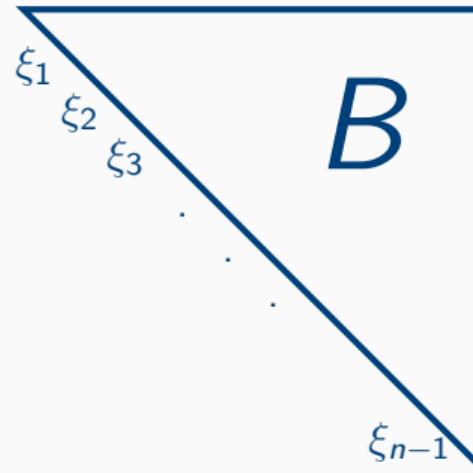
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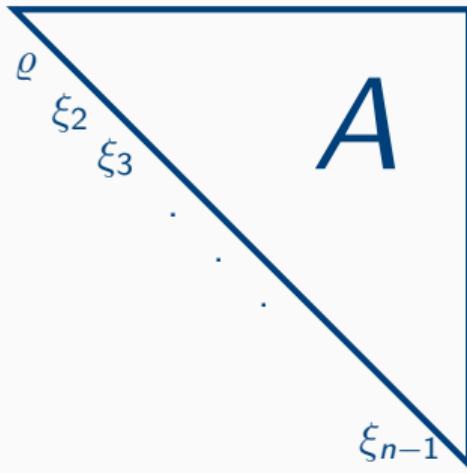
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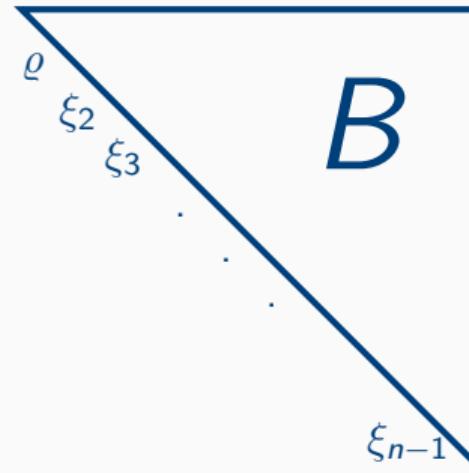
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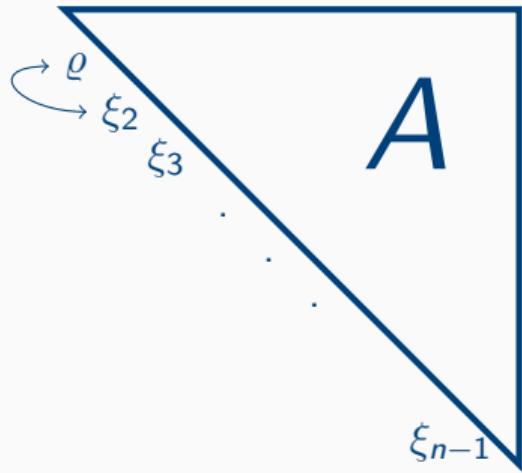
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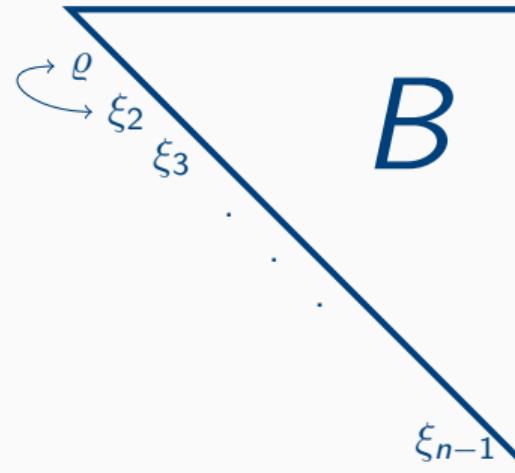
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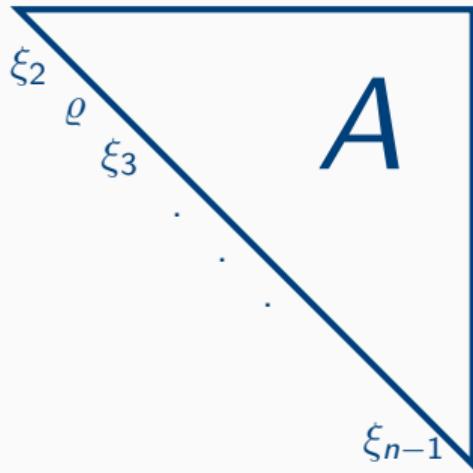
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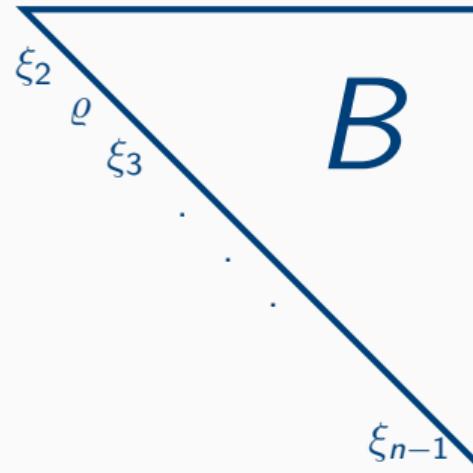
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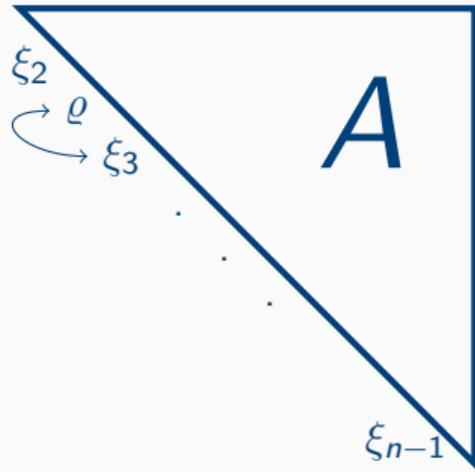
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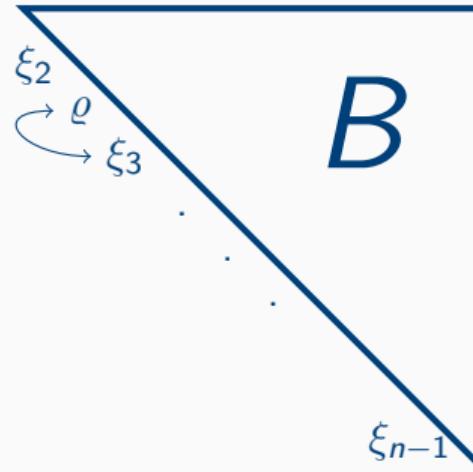
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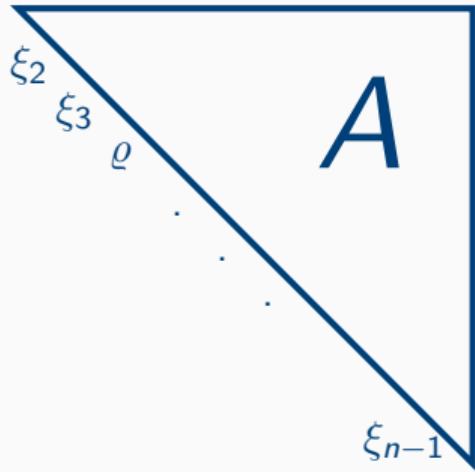
## A generalization: rational QZ



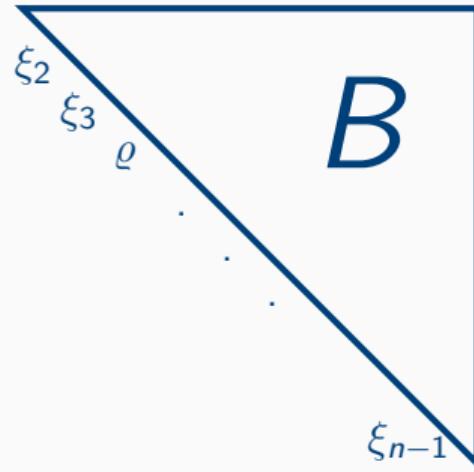
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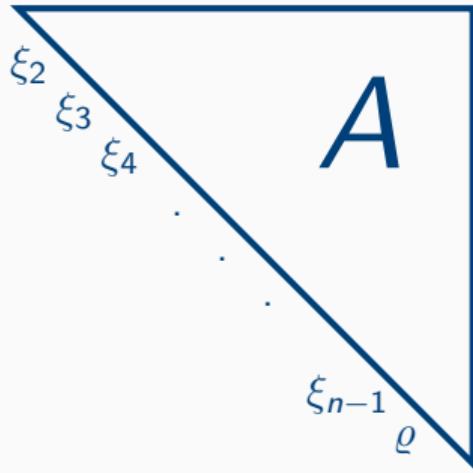
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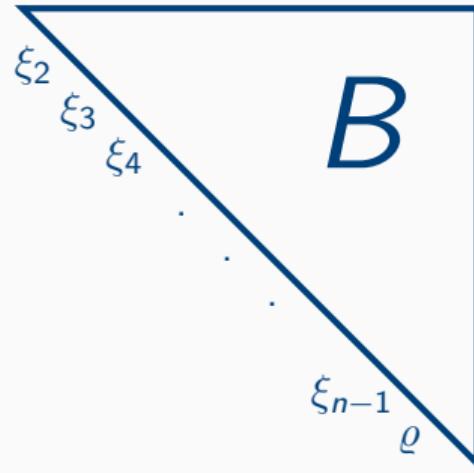
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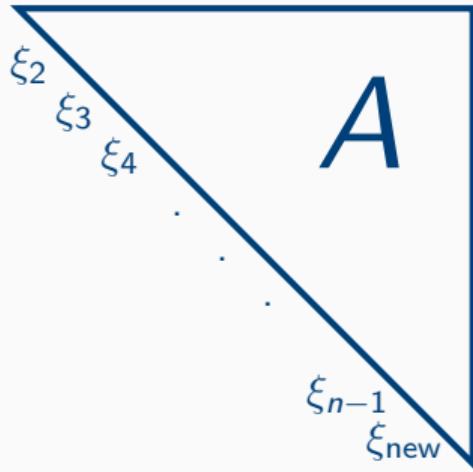
## A generalization: rational QZ



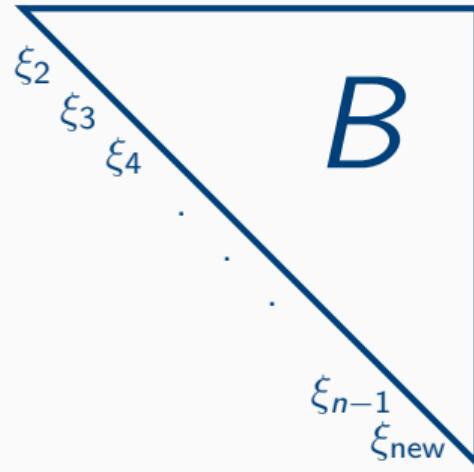
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## A generalization: rational QZ



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rational  $QZ$ : using the additional degrees of freedom

TODO

## Conclusion

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# Conclusion

- TODO

**Thank you**

## References

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