On the implicit restart of the rational Krylov method

Chasing algorithms for polynomial, extended and rational Krylov

Daan Camps, Karl Meerbergen, and Raf Vandebril

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

Problem statement

Problem setting

Single sentence problem statement

We want to compute a small number of eigenpairs of $A \in \mathbb{C}^{N \times N}$ that satisfy some property $\mathfrak{P}$.

Examples:

- All eigenvalues in a domain $\Omega \subset \mathbb{C}$
- The eigenvalue(s) with largest real part
- The eigenvalue(s) closest to the imaginary axis

Polynomial Krylov

Polynomial Krylov

Definition (Krylov subspace)

Given a matrix $A \in \mathbb{C}^{N \times N}$ and a vector $\mathbf{0} \neq \boldsymbol{v} \in \mathbb{C}^{N}$:

$$\mathcal{K}_{m+1} = \mathcal{K}_{m+1}(A, \boldsymbol{v}) := \operatorname{span}\{\boldsymbol{v}, A\boldsymbol{v}, \ldots, A^m \boldsymbol{v}\}.$$

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- Assumption: subspace is A-variant: $A\,\mathcal{K}_{m+1} \not\subseteq \mathcal{K}_{m+1}$.
- Isomorphism: $\mathcal{K}_{m+1} \cong \mathcal{P}_m$, i.e. $\forall \boldsymbol{w} \in \mathcal{K}_{m+1}, \exists p \in \mathcal{P}_m : \boldsymbol{w} = p(A)\boldsymbol{v}$ and vice versa.
- Orthogonal basis $V \in \mathbb{C}^{N\times(m+1)}$ such that

$$\text{span}\{V_{(:,1:k+1)}\} = \text{span}\{\boldsymbol{v}, A\boldsymbol{v}, \dots, A^k\boldsymbol{v}\} \qquad \forall k \leq m.$$

Polynomial Krylov

Arnoldi's method: recurrence relation

$$A\,V_m = V_m\,H_m + \,h_{m+1,m}\,v_{m+1}e_m^T$$

Polynomial Krylov

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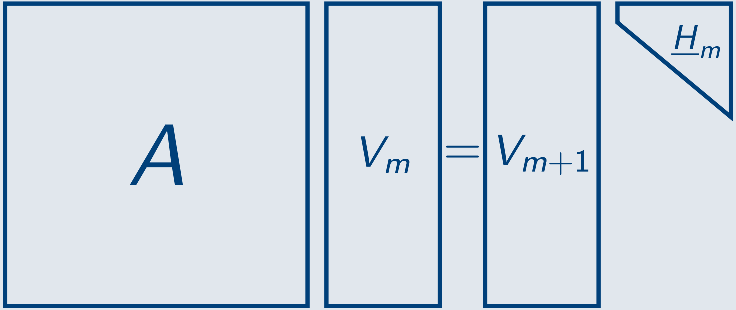
Arnoldi's method: recurrence relation



Polynomial Krylov

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

Polynomial Krylov

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

Small scale eigenvalue problem:

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

Ritz pairs $(\vartheta, \boldsymbol{x}) := (\vartheta, V_m \boldsymbol{z})$ satisfy Galerkin condition $A\boldsymbol{x} - \vartheta \boldsymbol{x} \perp \mathcal{K}_m$

Polynomial Krylov

What if the eigenvalues of A that satisfy $\mathfrak{P}$ only converge for $m \to N$?

Polynomial Krylov

What if the eigenvalues of A that satisfy $\mathfrak{P}$ only converge for $m \to N$?

- **Explicit restart:** for certain maximal m, select $\boldsymbol{w} \in \mathcal{K}_{m+1}$ and continue constructing new $\mathcal{K}_{m+1}(A, \boldsymbol{w})$ from scratch (Saad, 1980).
- **Implicit restart:** for certain maximal m, apply l-th order *polynomial filter* and continue from k-th order $\mathcal{K}_{k+1}(A, \hat{\boldsymbol{v}})$ $(l + k = m)$ (Sorensen, 1992).
- **Krylov-Schur:** compute and reorder the Schur decomposition of H_m (Stewart, 2001).

Polynomial Krylov

Implicitly restarted Arnoldi (IRA)

Input: $(V_{m+1}, \underline{H}_m), \{\varrho_i\}_{i=1}^{l}$

1: **for** $i = 1 \dots l$ **do**

2: $\quad \underline{H}_{m-i+1} - \varrho_i \underline{I}_{m-i+1} = \begin{bmatrix} Q & q \end{bmatrix} \begin{bmatrix} R \\ 0 \end{bmatrix}$

3: $\quad \underline{H}_{m-i} := Q^* \underline{H}_{m-i+1} Q_{(1:m-i+1,1:m-i)}$

4: $\quad V_{m-i+1} := V_{m-i+2} Q$

5: **end for**

6: **return** $\hat{V}_{k+1} := V_{k+1}, \hat{\underline{H}}_k := \underline{H}_k$

Polynomial Krylov

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6: **return** $\hat{V}_{k+1} := V_{k+1}, \underline{\hat{H}}_k := \underline{H}_k$

Result: $\hat{V}_{k+1} \boldsymbol{e}_1 = \prod_{i=1}^{l} (A - \varrho_i I) \boldsymbol{v}$

Polynomial Krylov

Practical implementation: Implicit-Q theorem

The Arnoldi decomposition $(V_{m+1}, \underline{H}_m)$ of order m is uniquely[1] defined by the matrix A and first column $V\boldsymbol{e}_1$.

[1] *essential uniqueness*

Polynomial Krylov

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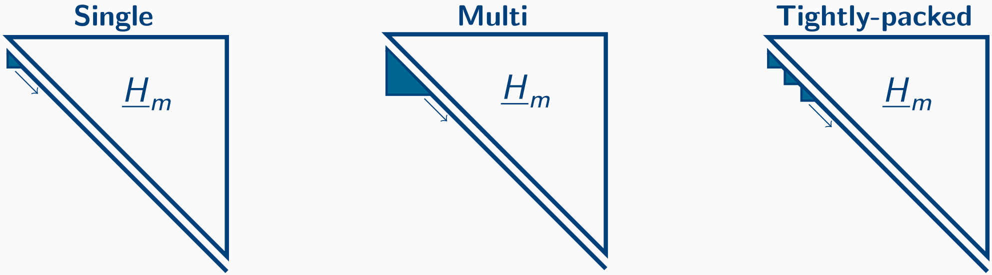

[1] *essential uniqueness*

Polynomial Krylov

Illustrative example

$A \in \mathbb{R}^{500\times 500}$, $\Lambda(A) \subset [0,1]$, $\mathfrak{P}$: rightmost eigenvalue

Diagonal matrix, logarithmically spaced eigenvalues

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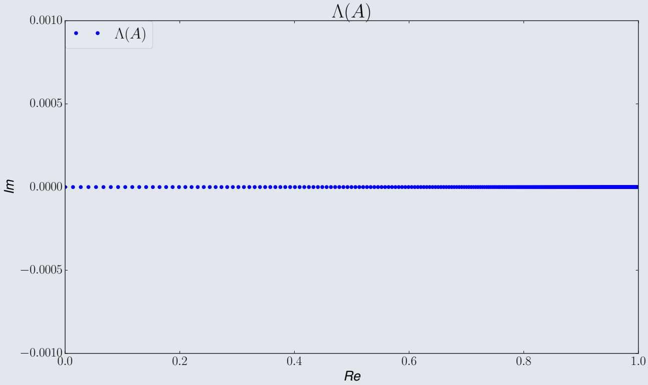
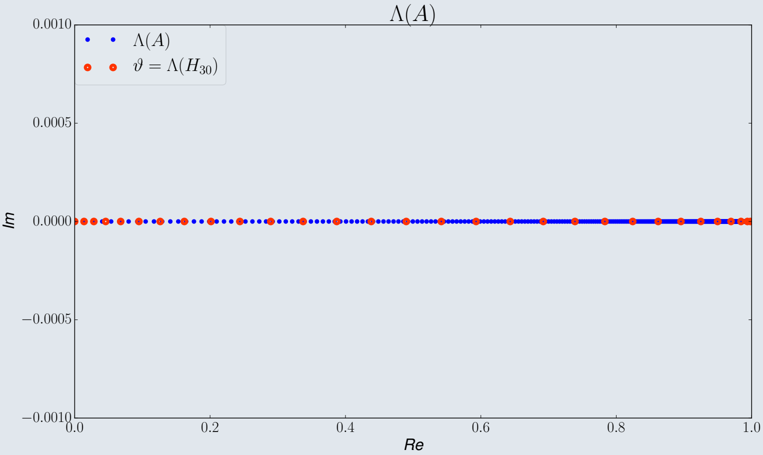


Polynomial Krylov

Illustrative example



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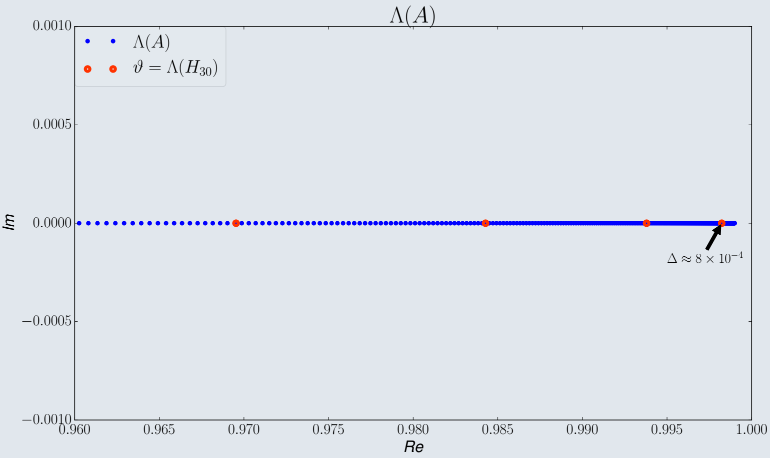

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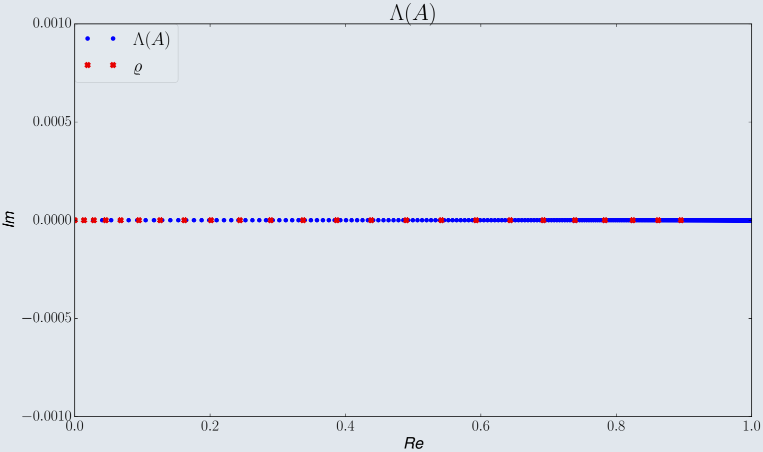

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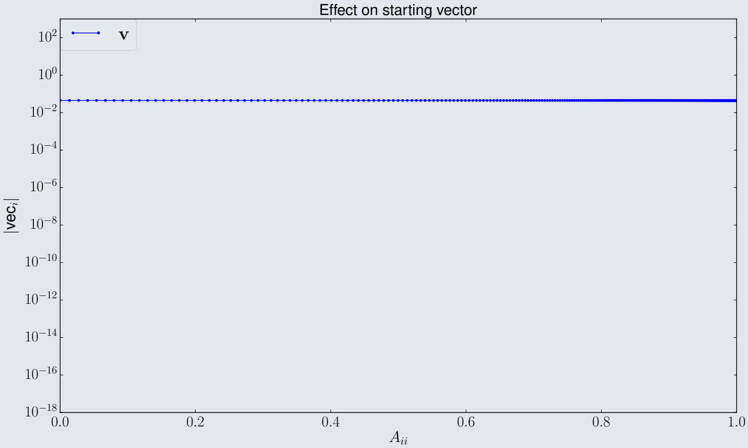

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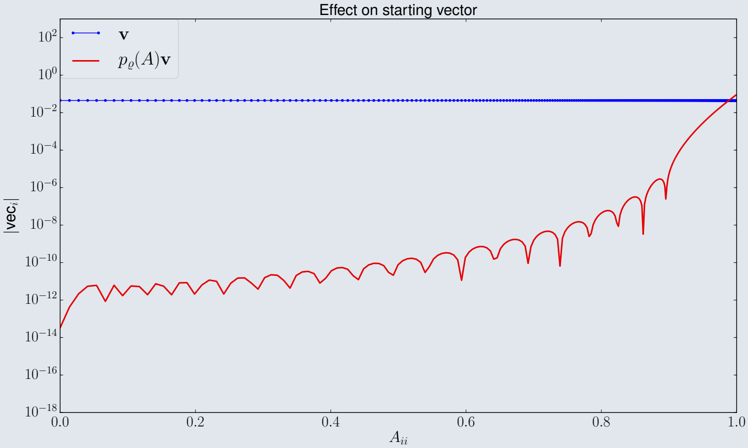

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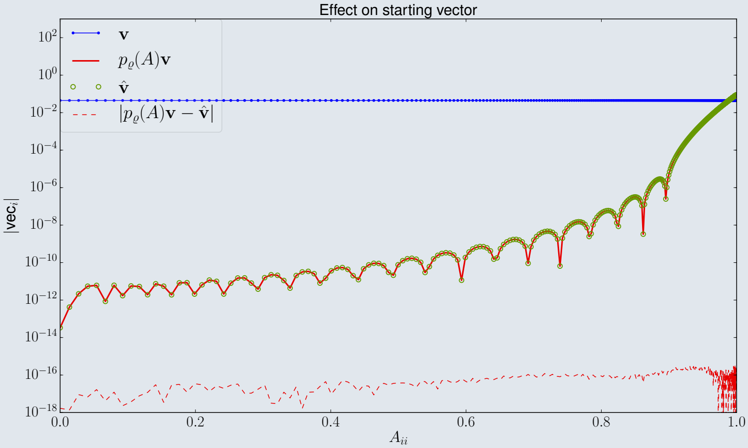

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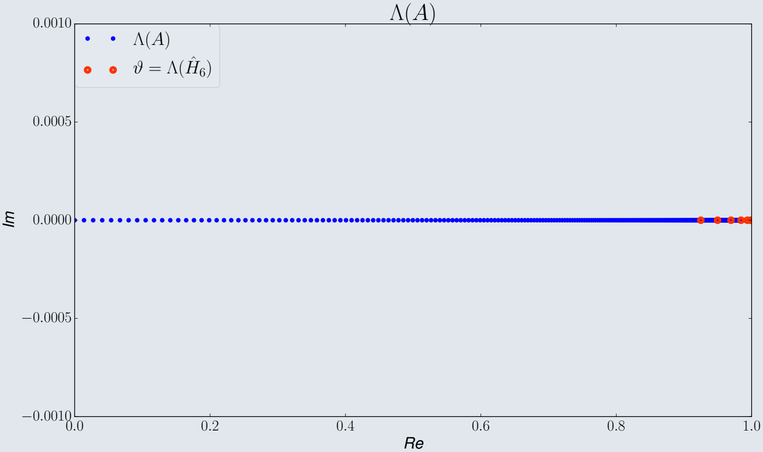

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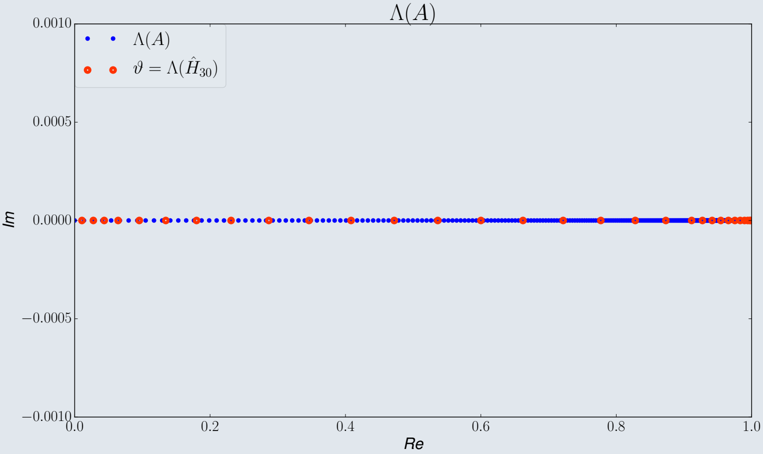

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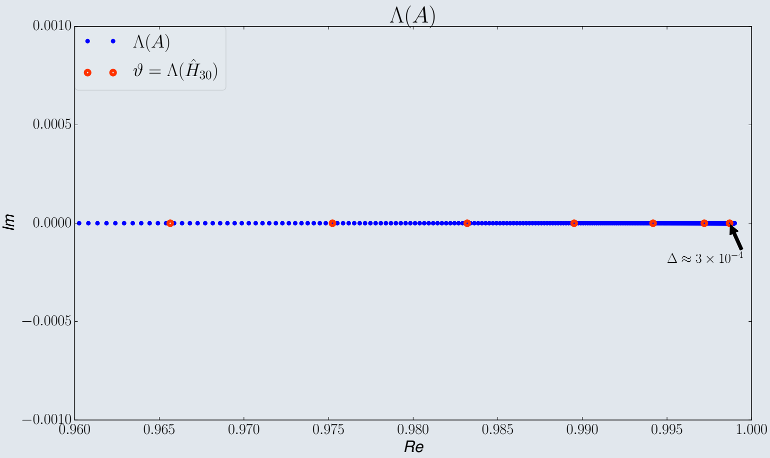

Rational Krylov

Rational Krylov

Definition (Rational Krylov sequence (Berljafa and Güttel, 2015))

Given a matrix $A \in \mathbb{C}^{N\times N}$, a vector $\mathbf{0} \neq \boldsymbol{v} \in \mathbb{C}^N$ and $q_m \in \mathcal{P}_m$ with roots $\Xi = \{\xi_1, \ldots, \xi_m\} \in \overline{\mathbb{C}} \setminus \Lambda(A)$:

$$\mathcal{Q}_{m+1}(A, \boldsymbol{v}, \Xi) = \mathcal{Q}_{m+1}(A, \boldsymbol{v}, q_m) := q_m(A)^{-1}\,\mathcal{K}_{m+1}(A, \boldsymbol{v}).$$

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Isomorphism: $\mathcal{Q}_{m+1} \cong q_m(z)^{-1}\mathcal{P}_m$, i.e. $\forall \boldsymbol{w} \in \mathcal{Q}_{m+1}, \exists \boldsymbol{p} \in \mathcal{P}_m : \boldsymbol{w} = q_m(A)^{-1}p(A)\boldsymbol{v}$

Rational Krylov

Rational Arnoldi's method (Ruhe, 1998): recurrence relation

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Rational Krylov

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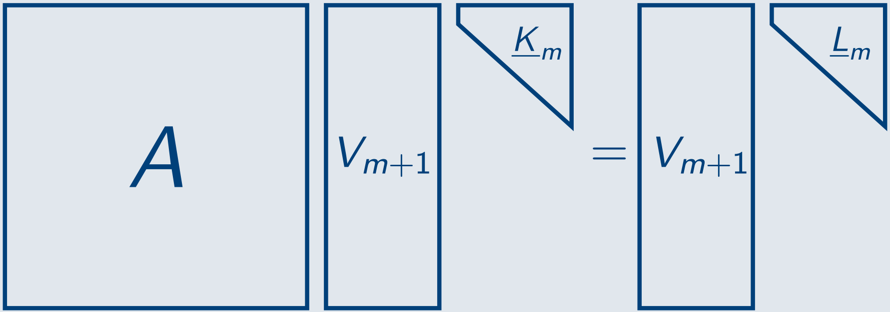

Rational Krylov

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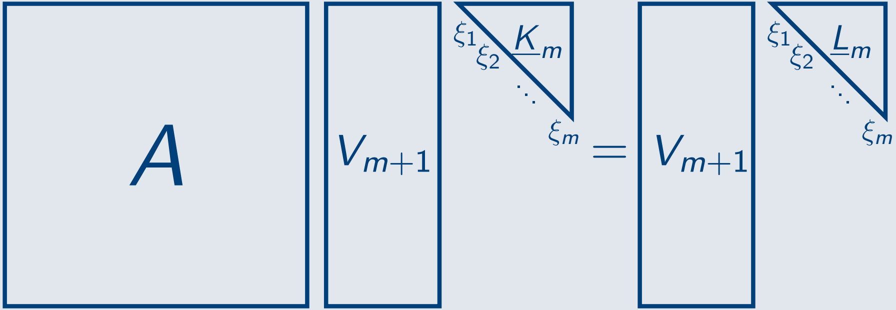

Rational Krylov

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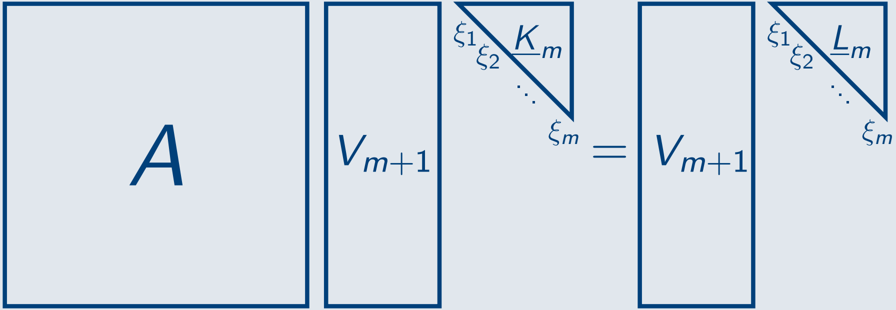

*(Abuse of) notation: $l_{i+1,i}/k_{i+1,i} = \xi_i$

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$A \, \boldsymbol{x} - \vartheta \, \boldsymbol{x} \perp \mathcal{K}_m(A, q_m(A)^{-1} \boldsymbol{v})$

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Rational Krylov

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Same solutions as before!

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- **Krylov-Schur:** compute and reorder the generalized Schur decomposition of (L_m, K_m) (De Samblanx et al., 1997).

Rational Krylov

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Special case: extended Krylov introduced by Druskin and Knizhnerman (1998)

$$\Xi_{\text{ext}} = \{\xi_i\}_{i=1}^{m}, \forall i : \xi_i \in \{0, \infty\}$$

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Example: $\Xi_{\text{ext}} = \{0, \infty, \ldots, 0\}$

The matrix pencil is in *condensed* format, chasing by elementary unitary operations (Camps et al., 2016)

Rational Krylov

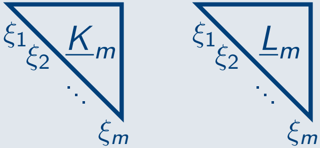
How to apply the polynomial filter implicitly?

General case:

No longer in condensed format!

Rational Krylov

Solution



Rational Krylov

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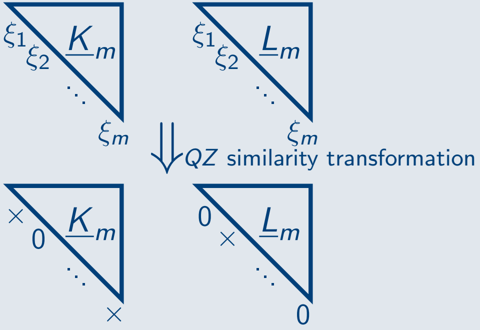

Rational Krylov

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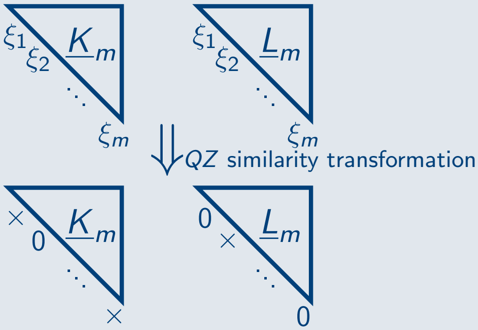
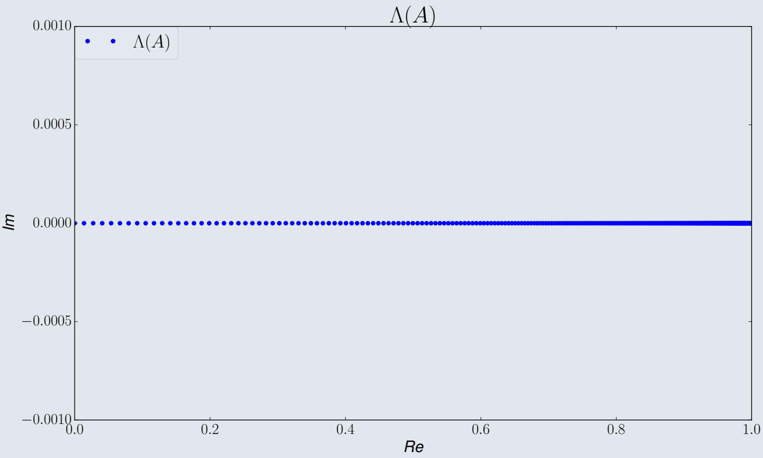


The QZ transformation is formulated in terms of elementary transformations on core transformations

Rational Krylov

Illustrative example



Rational Krylov

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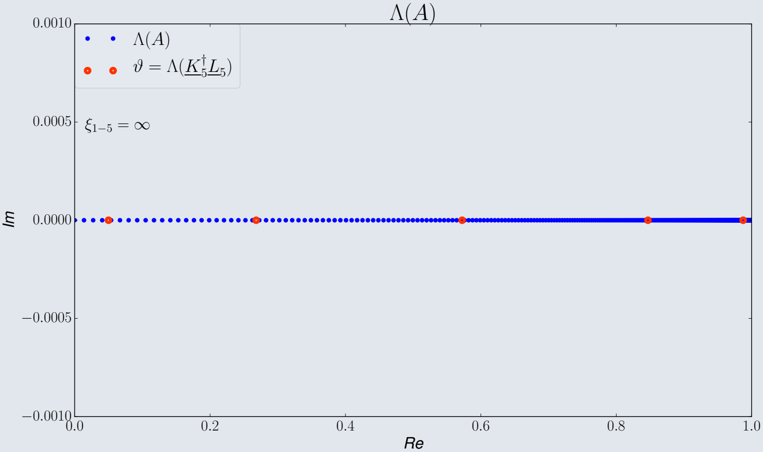

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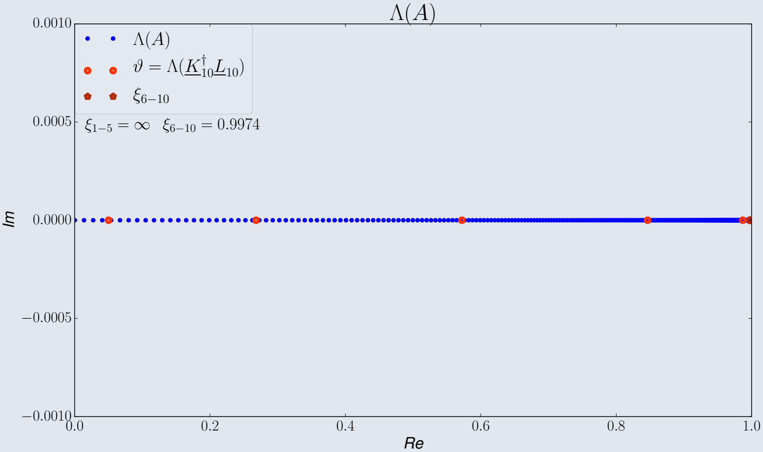

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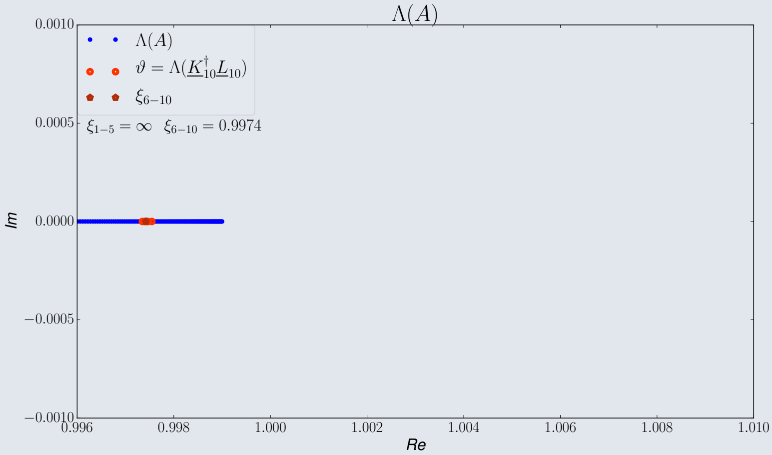

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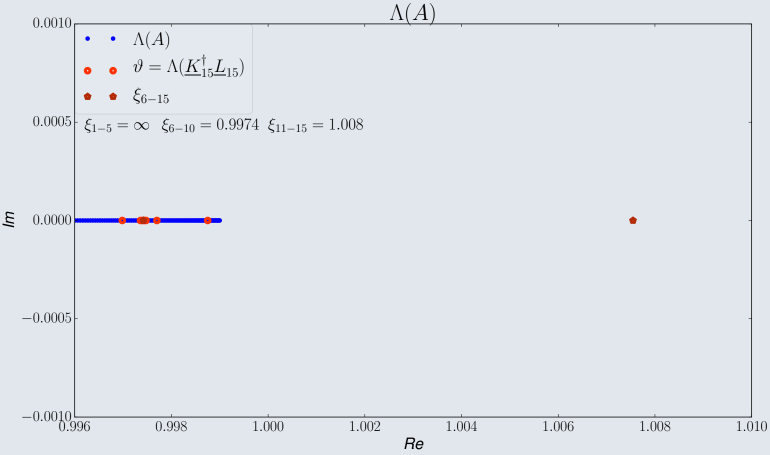

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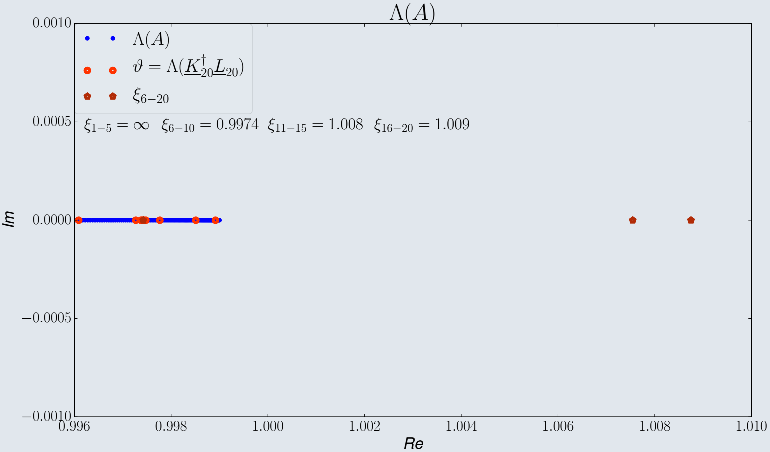

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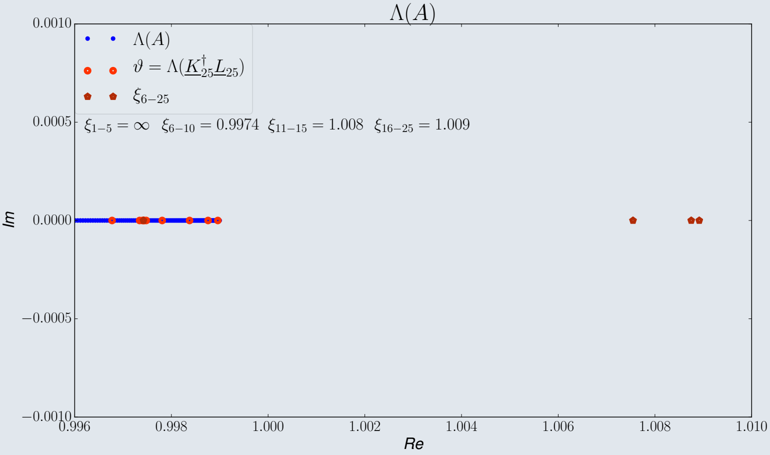

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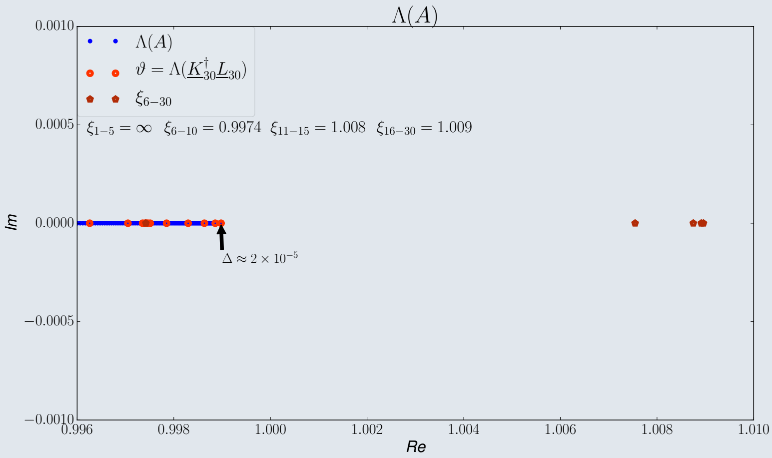

Rational Krylov

Illustrative example

Transformation: $(V_{m+1}, \underline{K}_m, \underline{L}_m) \rightarrow (\tilde{V}_{m+1}, \underline{\tilde{K}}_m, \underline{\tilde{L}}_m)$ with $\Xi_{\text{ext}} = \{\infty, 0, \infty, 0, \ldots, 0\}$

Rational Krylov

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$$\mathcal{Q}_{m+1}(A, \boldsymbol{v}, q_m) = \tilde{\mathcal{Q}}_{m+1}(A, \boldsymbol{w}, \Xi_{\text{ext}}) \quad \Rightarrow \quad \boldsymbol{w} = \alpha\, q_m(A)^{-1} A^{m/2}\, \boldsymbol{v}$$

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Ritz values are **not** affected: $\underline{\tilde{K}}_m = Q\, \underline{K}_m\, Z, \quad \underline{\tilde{L}}_m = Q\, \underline{L}_m\, Z$

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$$\underline{\tilde{K}}_m^{\dagger} \underline{\tilde{L}}_m = Z^* \underline{K}_m^{\dagger} Q^* Q \underline{L}_m Z$$

Rational Krylov

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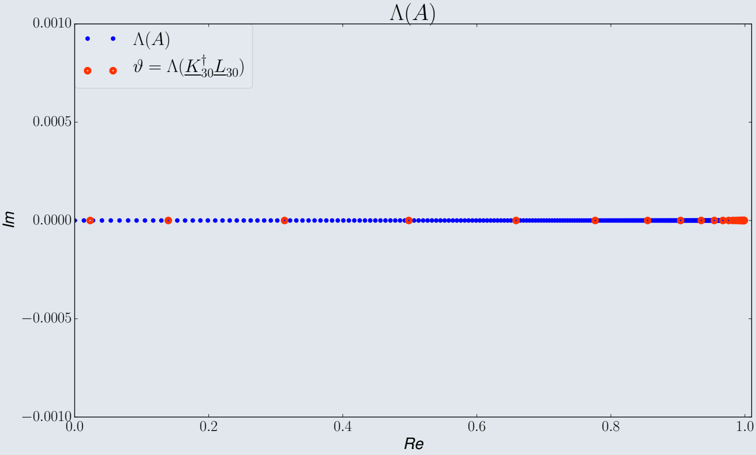

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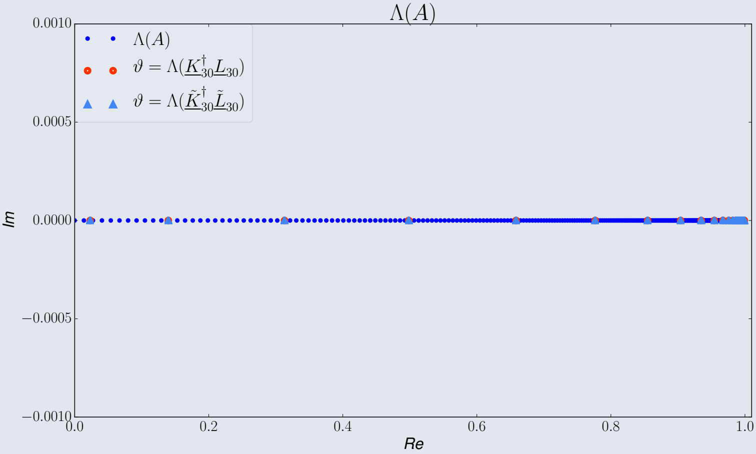

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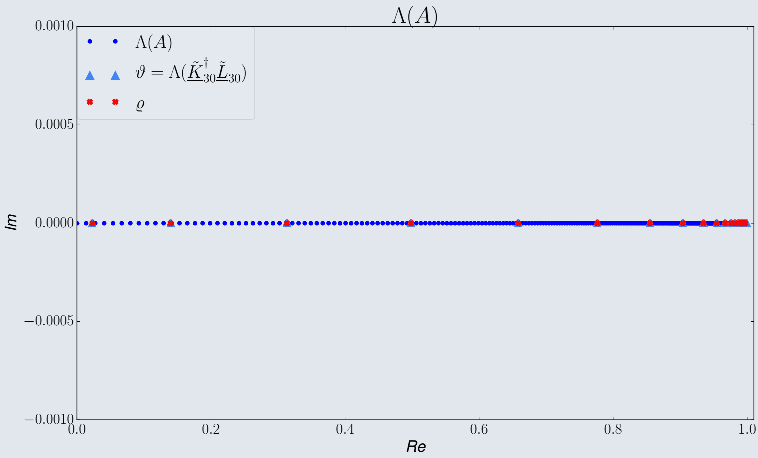

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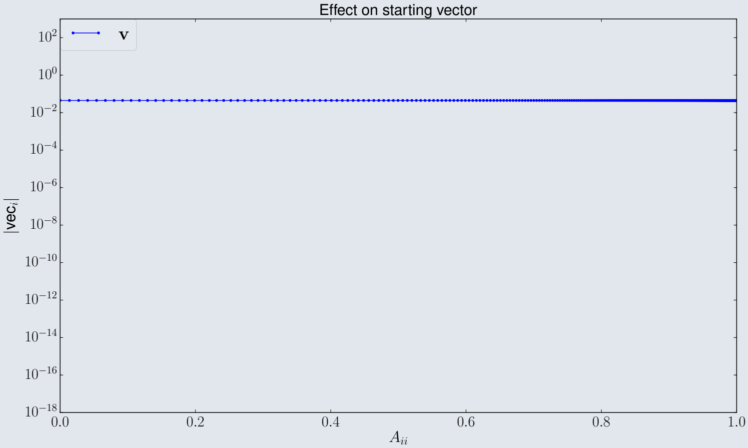

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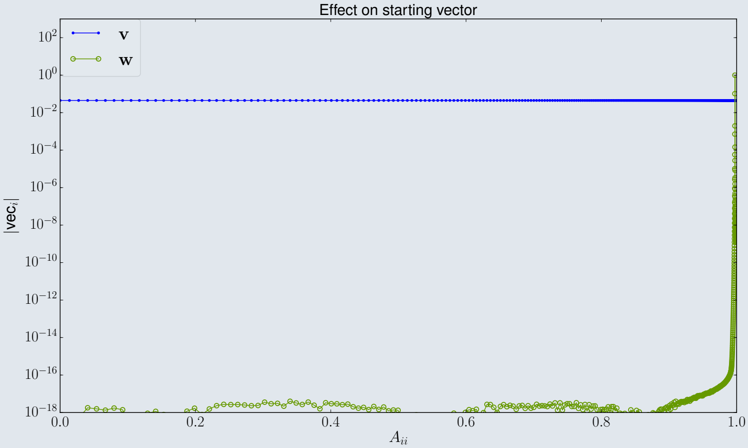

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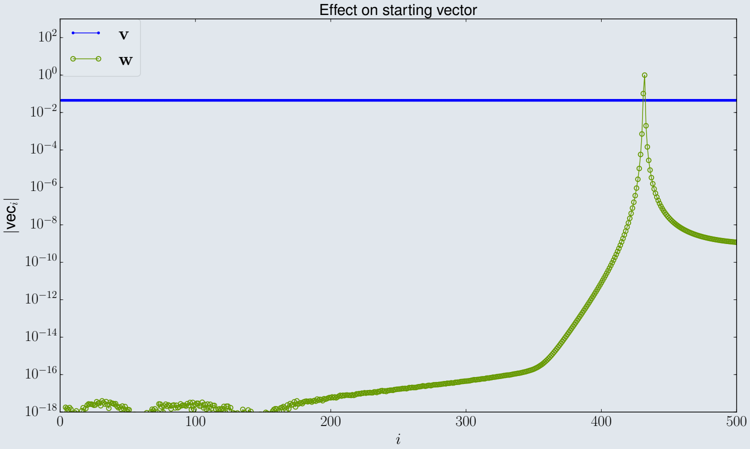

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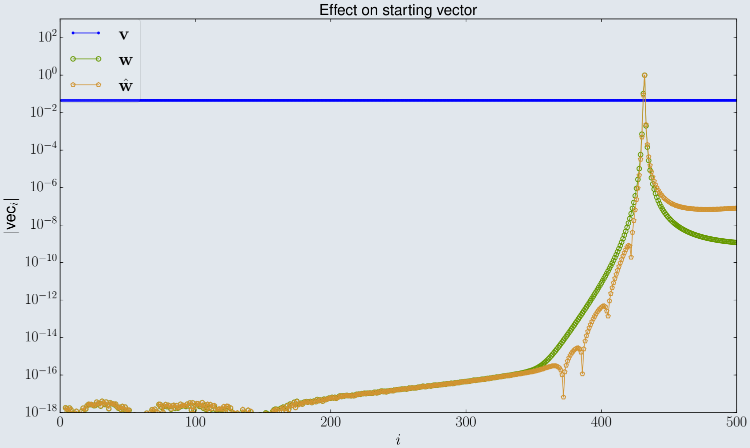

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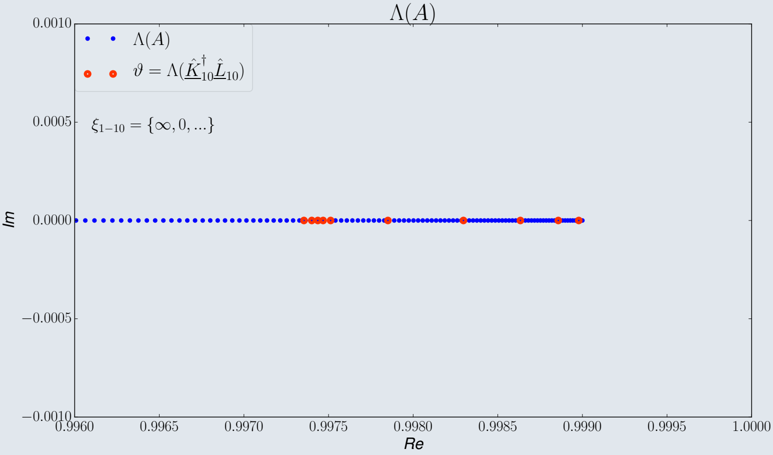

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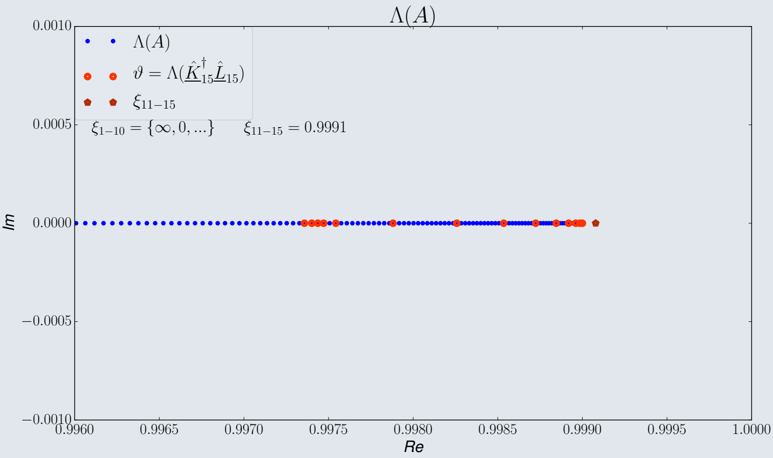

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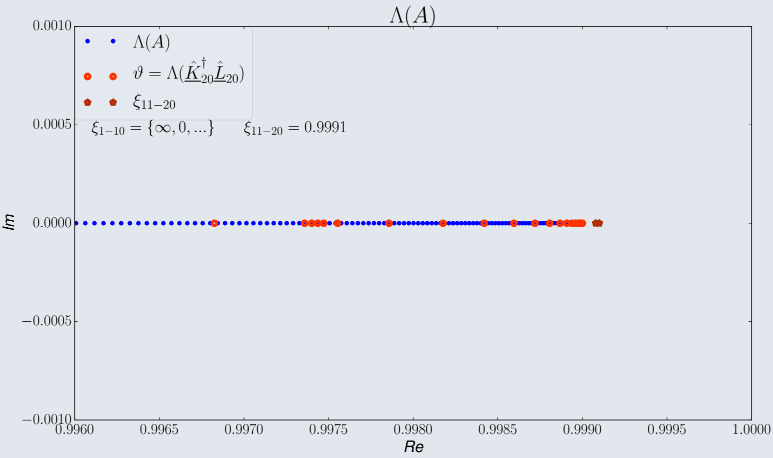

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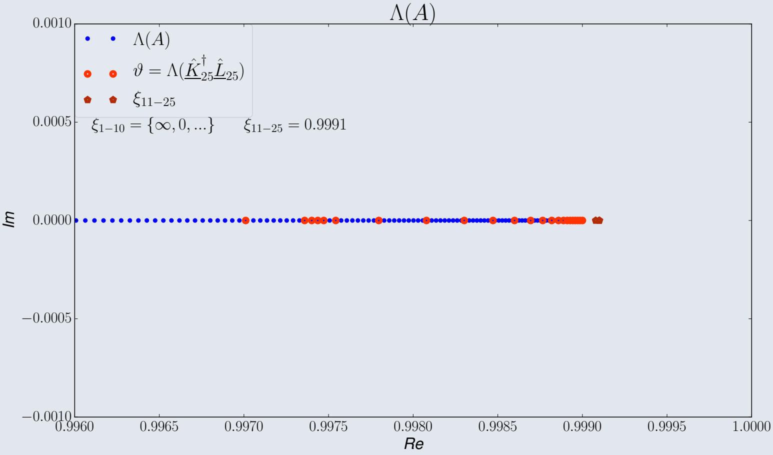
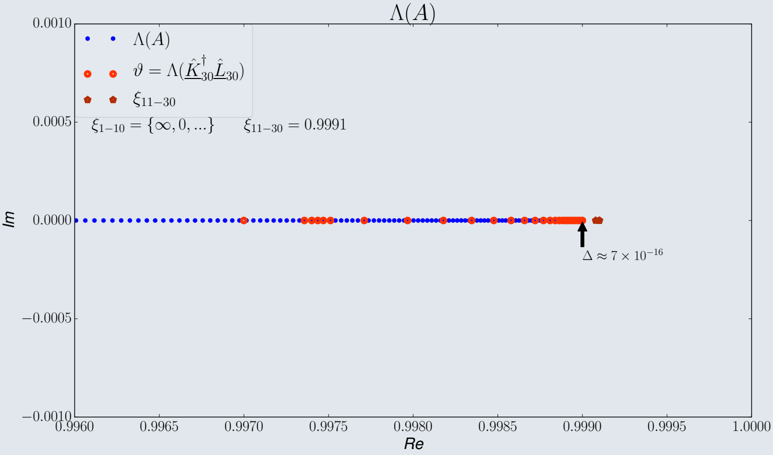


Rational Krylov

Illustrative example



Conclusion

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- Filtering (rational) Krylov subspaces is useful to limit subspace dimension when searching for eigenvalues satisfying a property $\mathfrak{P}$
- The filter can be applied implicitly by means of elementary unitary operations (*chasing*) both for polynomial and rational Krylov

Thank you

References

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