A rational Krylov method for a class of non-linear eigenvalue problems

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Motivation

- Solution of linear eigenvalue problem

$$Ax = \lambda Bx$$

  is pretty well understood
  - Appealing method: shift-and-invert Arnoldi
  - Reliable for computing several eigenvalues near a shift point.
  - Rational Krylov: more than one interpolation points = poles.
- Polynomial eigenvalue problems
  - We can use Krylov methods (when we 'linearize')

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- Polynomial eigenvalue problems
  - We can use Krylov methods (when we 'linearize')
- Solution of non-linear eigenvalue problem

$$A(\lambda)x = 0$$

  - Residual inverse iteration and Newton iterations are locally convergent methods
  - Globally convergent methods by using polynomial approximation of $A(\lambda)$

Outline

1. Motivation
2. Polynomial eigenvalue problem
3. Nonlinear eigenvalue problem
4. Rational Krylov

Linearization for polynomial eigenvalue problems

- Quadratic eigenvalue problem:

$$Kx + \lambda Cx + \lambda^2 Mx = 0$$

- Transform the problem to

$$\begin{aligned} Ax &= \lambda Bx \\ \begin{bmatrix} K & C \\ 0 & I \end{bmatrix} \begin{pmatrix} x \\ \lambda x \end{pmatrix} &= \lambda \begin{bmatrix} 0 & -M \\ I & 0 \end{bmatrix} \begin{pmatrix} x \\ \lambda x \end{pmatrix} \end{aligned}$$

- Many papers: [Tisseur, 2000], [Mackey, Mackey, Mehl, Mehrmann 2006], ...
- Is a linear problem, so we can use Arnoldi's method
- At first sight: doubling the size requires double memory cost, but this is not the case

Polynomial eigenvalue problem

- Polynomial eigenvalue problem:

$$A_0x + \lambda A_1x + \cdots + \lambda^N A_N x = 0$$

- Transformed to

$$\left(\begin{bmatrix} A_0 & A_1 & \cdots & A_{p-1} \\ & I & & \\ & & \ddots & \\ & & & I \end{bmatrix} - \lambda \begin{bmatrix} 0 & \cdots & \cdots & -A_N \\ I & & & 0 \\ & \ddots & & \vdots \\ & & I & 0 \end{bmatrix} \right) \begin{bmatrix} x \\ \lambda x \\ \vdots \\ \lambda^{p-1}x \end{bmatrix} = 0$$

Linearization for polynomial eigenvalue problems

- Shift-and-invert transform $(A-\sigma B)^{-1}B$:

$$\lambda^{-1}\begin{pmatrix} x \\ \lambda x \\ \vdots \\ \lambda^{p-1}x \end{pmatrix} = \begin{bmatrix} S_1 & \cdots & \cdots & S_p \\ I & & & 0 \\ & \ddots & & \vdots \\ & & I & 0 \end{bmatrix}\begin{pmatrix} x \\ \lambda x \\ \vdots \\ \lambda^{p-1}x \end{pmatrix}$$

- Krylov sequence:

$$\begin{pmatrix} v \\ 0 \\ \vdots \end{pmatrix}$$

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$$\begin{pmatrix} v \\ 0 \\ \vdots \end{pmatrix} \qquad \begin{pmatrix} w = S_1 v \\ v \\ 0 \\ \vdots \end{pmatrix}$$

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- Krylov sequence:

$$\begin{pmatrix} v \\ 0 \\ \vdots \end{pmatrix} \quad \begin{pmatrix} w \\ v \\ 0 \\ \vdots \end{pmatrix} \quad \begin{pmatrix} t = S_1 w + S_2 v \\ w \\ v \\ 0 \\ \vdots \end{pmatrix}$$

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- Krylov sequence:

$$\begin{pmatrix} v \\ 0 \\ \vdots \end{pmatrix} \quad \begin{pmatrix} w \\ v \\ 0 \\ \vdots \end{pmatrix} \quad \begin{pmatrix} t \\ w \\ v \\ 0 \\ \vdots \end{pmatrix} \quad \begin{pmatrix} u = S_1 t + S_2 w + S_3 v \\ t \\ w \\ v \\ 0 \\ \vdots \end{pmatrix}$$

Linearization for polynomial eigenvalue problems

- Shift-and-invert transform:

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- Krylov sequence:

$$\begin{pmatrix} v_1 & v_2 & v_3 & v_4 & \cdots & v_k \\ 0 & v_1 & v_2 & v_3 & & v_{k-1} \\ \vdots & 0 & v_1 & v_2 & & v_{k-2} \\ & \vdots & 0 & v_1 & & \vdots \\ & & \vdots & 0 & & \vdots \\ & & & \vdots & & v_1 \\ & & & & & 0 \end{pmatrix}$$

Nonlinear eigenvalue problem

- Straightforward idea: choose an approximation of a fixed degree and solve the corresponding polynomial eigenvalue problem:
  - Polynomial expansion, e.g. Taylor, Chebyshev, ...

$$A(\lambda) \approx A_0 p_0(\lambda) + \cdots + A_N p_N(\lambda)$$

    [Amiraslani, Corless, Lancaster, 2009], [Effenberger, Kressner, 2011]
  - Rational expansion, e.g. (Chebyshev) Padé

$$A(\lambda) \approx A_0 \frac{\alpha_0}{\lambda - \sigma_0} + \cdots + A_N \frac{\alpha_N}{\lambda - \sigma_N}$$

    [Su & Bai, 2011]
  - Spectral discretization

$$A(\lambda) \approx A_0 + \lambda \frac{A_0 p_0(\lambda) + \cdots + A_N p_N(\lambda)}{\alpha_0 p_0(\lambda) + \cdots + \alpha_N p_N(\lambda)}$$

    [Trefethen 2000], [Michiels, Niculescu 2007],
    [Breda, Maset, Vermiglio 2005]
- In this talk, we explore a 'flexible' choice of N and p_j.

Taylor-Arnoldi

- [Jarlebring, Meerbergen, Michiels, 2010]
- Power sequence on Taylor series

$$A(\lambda) \approx A_0 + \lambda A_1 + \lambda^2 A_2 + \cdots$$

- For k iterations of Arnoldi, use Companion linearization with $N > k$
- Arnoldi:

$$\begin{pmatrix} v \\ 0 \\ \vdots \end{pmatrix}$$

- Breakthrough for solving the delay (equation) eigenvalue problem

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$$\begin{pmatrix} v \\ 0 \\ \vdots \end{pmatrix} \quad \begin{pmatrix} w \\ v \\ 0 \\ \vdots \end{pmatrix} \quad \begin{pmatrix} t = -A_0^{-1}(A_1 w + A_2)v \\ w \\ v \\ 0 \\ \vdots \end{pmatrix}$$

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Other polynomials

- Use polynomials in order to
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- Lagrange polynomial
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- A (partly) successful generalization of Taylor-Arnoldi to rational Krylov

Newton polynomial basis

- Newton polynomials:

$$N_0 := 1, N_1 := (\lambda - \sigma_0), N_2 := (\lambda - \sigma_0)(\lambda - \sigma_1), \ldots$$

- $A(\lambda) = A_0 N_0 + A_1 N_1 + \cdots$ with
  - $A_0 = [A_0] = A(\sigma_j)$ and
  - $A_j = [A_0, \ldots, A_j] = \dfrac{[A_1, \ldots, A_j] - [A_0, \ldots, A_{j-1}]}{\sigma_j - \sigma_0}$ (divided difference).
- $\sigma_0, \sigma_1, \ldots$ are interpolation points.
- Linearization:

$$\left(\begin{bmatrix} A_0 & A_1 & & \cdots & A_N \\ \sigma_0 I & I & & & \\ & \sigma_1 I & I & & \\ & & \ddots & \ddots & \\ & & & \sigma_{N-2} I & I \end{bmatrix} - \lambda \begin{bmatrix} 0 & \cdots & \cdots & 0 \\ I & & & \vdots \\ & \ddots & & \vdots \\ & & I & 0 \end{bmatrix} \right) \begin{bmatrix} x \\ N_1(\lambda)x \\ N_2(\lambda)x \\ \vdots \\ \vdots \end{bmatrix} = 0$$

- $A^{-1}B$ is not a block upper Hessenberg matrix

Rational Krylov

- Shift-and-invert step: $(A - \sigma_j B)w = Bv$
- First step: multiply by B: shift vector downwards

$$B \cdot v = w$$

$$\begin{bmatrix} 0 & \cdots & \cdots & 0 \\ I & & & \vdots \\ & \ddots & & \vdots \\ & & I & 0 \end{bmatrix} \cdot \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_{N-1} \\ v_N \end{bmatrix} = \begin{bmatrix} 0 \\ v_1 \\ v_2 \\ \vdots \\ v_{N-1} \end{bmatrix}$$

- Then apply $(A - \sigma_j B)^{-1}$:

$$A - \sigma_j B = \begin{bmatrix} A_0 & A_1 & & \cdots & A_N \\ (\sigma_0 - \sigma_j)I & I & & & \\ & (\sigma_1 - \sigma_j)I & I & & \\ & & \ddots & \ddots & \\ & & & (\sigma_{N-1} - \sigma_j)I & I \end{bmatrix}$$

Rational Krylov

- $\mu_i^j = \sigma_i - \sigma_j$.
- Shift-and-invert-step:

$$\begin{bmatrix} A_0 & A_1 & A_2 & A_3 & A_4 & A_5 \\ \sigma_1 I & I & & & & \\ & \sigma_2 I & I & & & \\ & & \sigma_3 I & I & & \\ & & & \sigma_4 I & I & \\ & & & & \sigma_5 I & I \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ \star \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \star \\ \star \\ \star \\ \star \\ \star \\ \star \end{bmatrix}$$

- $(A - \sigma_j B)^{-1} B$ applied to v_j respects the desired zero structure in the vectors
- This is rational Krylov with poles $\sigma_1, \sigma_2, \ldots$
- Linear recurrence relation of the form:

$$AV_{k+1}\underline{H}_k = BV_{k+1}\underline{L}_k$$

Rational Krylov

- $\mu_i^j = \sigma_i - \sigma_j$.
- Shift-and-invert-step: $A - \sigma_1 B$

$$\begin{bmatrix} A_0 & A_1 & A_2 & A_3 & A_4 & A_5 \\ \mu_1^2 I & I & & & & \\ & 0 & I & & & \\ & & \mu_3^2 I & I & & \\ & & & \mu_4^2 I & I & \\ & & & & \mu_5^2 I & I \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ \star \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \star \\ \star \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

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Rational Krylov

- $\mu_i^j = \sigma_i - \sigma_j$.
- Shift-and-invert-step: $A - \sigma_2 B$

$$\begin{bmatrix} A_0 & A_1 & A_2 & A_3 & A_4 & A_5 \\ \mu_1^3 I & I & & & & \\ & \mu_2^3 I & I & & & \\ & & 0 & I & & \\ & & & \mu_4^3 I & I & \\ & & & & \mu_5^3 I & I \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ \star \\ \star \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \star \\ \star \\ \star \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

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Rational Krylov

- $\mu_i^j = \sigma_i - \sigma_j$.
- Shift-and-invert-step: $A - \sigma_3 B$

$$\begin{bmatrix} A_0 & A_1 & A_2 & A_3 & A_4 & A_5 \\ \mu_1^4 I & I & & & & \\ & \mu_2^4 I & I & & & \\ & & \mu_3^4 I & I & & \\ & & & 0 & I & \\ & & & & \mu_5^4 I & I \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ \star \\ \star \\ \star \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \star \\ \star \\ \star \\ \star \\ 0 \\ 0 \end{bmatrix}$$

- $(A - \sigma_j B)^{-1} B$ applied to v_j respects the desired zero structure in the vectors
- This is rational Krylov with poles $\sigma_1, \sigma_2, \ldots$
- Linear recurrence relation of the form:

$$AV_{k+1}\underline{H}_k = BV_{k+1}\underline{L}_k$$

Rational Krylov

- $\mu_i^j = \sigma_i - \sigma_j$.
- Shift-and-invert-step: $A - \sigma_4 B$

$$\begin{bmatrix} A_0 & A_1 & A_2 & A_3 & A_4 & A_5 \\ \mu_1^5 I & I & & & & \\ & \mu_2^5 I & I & & & \\ & & \mu_3^5 I & I & & \\ & & & \mu_4^5 I & I & \\ & & & & 0 & I \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ \star \\ \star \\ \star \\ \star \\ 0 \end{bmatrix} = \begin{bmatrix} \star \\ \star \\ \star \\ \star \\ \star \\ 0 \end{bmatrix}$$

- $(A - \sigma_j B)^{-1} B$ applied to v_j respects the desired zero structure in the vectors
- This is rational Krylov with poles $\sigma_1, \sigma_2, \ldots$
- Linear recurrence relation of the form:

$$AV_{k+1}\underline{H}_k = BV_{k+1}\underline{L}_k$$

Rational Krylov

- With constant continuation vector

$$v_1, (A - \sigma_1 B)^{-1} B v_1, (A - \sigma_2 B)^{-1} B v_1, \ldots$$

- On each iteration, we must solve the system:

$$A(\sigma_j) w_j = [A(\sigma_0), A(\sigma_j)] v_1$$

  So, only two matrices have to be stored: $A(\sigma_0)$ and $A(\sigma_j)$.
- Note: $[A(\sigma_0), A(\sigma_j)] \approx A'(\sigma_j)$
- Recurrence relation has small residual norm (rounding errors).
- Caveat: choice of continuation vector may be unstable.
  When the σ_j become Ritz values or converged Ritz value show up again, be worried.

Rational Krylov

- Usual choice of continuation vector

$$v_1, (A - \sigma_1 B)^{-1} B v_1, (A - \sigma_2 B)^{-1} B v_2, \ldots$$

  where v_j is the last subspace vector.
- On each iteration, we must solve the system:

$$A(\sigma_j) w_j = \sum_{i=1}^{j} A_i w_{j-1,i}$$

  So, k divided differences have to be stored or computed
- Note: $\sum_{i=1}^{j} A_i w_{j-1,i} \approx A'(\sigma_j) w_{0,i}$
- Recurrence relation has small residual norm (rounding errors).
- Is known to be stable in practice.

Lagrange polynomial basis

- Lagrange polynomials:

$$L_j := \omega_j \prod_{i \neq j} (\lambda - \sigma_i) \quad , \quad \omega_j = \left(\prod_{i \neq j} (\sigma_j - \sigma_i) \right)^{-1} \quad , \quad j = 0, \ldots, N$$

- $A(\lambda) = A_0 L_0 + A_1 L_1 + \cdots$ with
  - $A_j = A(\sigma_j)$, $j = 0, \ldots, N$ and
  - $\sigma_0, \sigma_1, \ldots$ the interpolation points.
- Linearization:

$$\left(\begin{bmatrix} A_0 & \cdots & A_N & 0 \\ \sigma_0 I & & & -\omega_0 \\ & \ddots & & \vdots \\ & & \sigma_{N-2} I & -\omega_N I \end{bmatrix} - \lambda \begin{bmatrix} 0 & \cdots & \cdots & 0 \\ I & & & \vdots \\ & \ddots & & \vdots \\ & & I & 0 \end{bmatrix} \right) \begin{bmatrix} L_0 x \\ L_1 x \\ \vdots \\ L_N x \end{bmatrix} = 0$$

- $A^{-1}B$ is not a block upper Hessenberg matrix

Rational Krylov

- Apply shift: $(A - \sigma_j B)u = \lambda B u$ has the following form:

$$\left(\left[\begin{array}{c|c|ccc} A_0 & A_1 & \cdots & A_N & 0 \\ \star & & & & -\omega_0 I \\ \hline & 0 & & & \vdots \\ \hline & & \ddots & & \\ & & & \star & -\omega_N I \end{array}\right] - \lambda \left[\begin{array}{c|c|ccc} 0 & \cdots & \cdots & & 0 \\ I & & & & 0 \\ \hline & I & & & 0 \\ \hline & & & \ddots & \vdots \\ & & & I & 0 \end{array}\right] \right) \begin{bmatrix} x \\ L_1 x \\ L_2 x \\ \vdots \\ L_N x \end{bmatrix} = 0$$

- $(A - \sigma_j B)^{-1} B$ applied to v_j respects the desired zero structure in the vectors
- For constant continuation vector, only A_0 and A_j need to be stored, but risk of numerical instabilities.
- For classical continuation vector, all interpolation matrices need to be stored.

Chebyshev series

- $A(\lambda) = A_0 T_0 + A_1 T_1 + \cdots$
- Linearization:

$$\left(\begin{bmatrix} -A_0 & -A_1 & & \cdots & \star \\ 0 & I & & & \\ I & 0 & I & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & I \\ & & & I & 0 \end{bmatrix} - \lambda \begin{bmatrix} 0 & \cdots & \cdots & \cdots & -A_N \\ I & & & & 0 \\ & 2I & & & 0 \\ & & \ddots & & \vdots \\ & & & 2I & 0 \end{bmatrix} \right) x = 0$$

- No block upper Hessenberg structure
- Arnoldi iterations require computation of $A(0)$, $A'(0)$ expressed in Chebyshev basis.
- i.e. moment matching requires the full Chebyshev expansion (use a functional framework [Jarlebring, Michiels, M. 2011])
- Shifting as for Newton basis does not help.

Numerical example: Hopf bifurcation

- Nonlinear equation: $\dot{x} = f(x, \lambda)$
- Hopf bifurcation of dynamical system: $A(\lambda)u = i\mu u$ with μ real
- λ is an eigenvalue of $(A(\lambda) \otimes I + I \otimes A(\lambda)x = 0$
- Usually: continuation method for λ
- Modified Olmstead model ($n = 40$) of the form:

$$(A + \lambda E_u + (\lambda + 1)^{-1} E_u + (\lambda + 2)^{-1/2} E_v)u = 0$$

- Pick ten poles in a Leja fashion in $[6, 10]$, then use Ritz value.
- For related work, see
  [Guckerheimer et al. 1993, 1997], [Govaerts, 2000]
  [M. & Spence 2010], [Elman, M., Spence, Wu, 2012]

Hopf bifurcations

- Constant continuation vector:
  - Maximum one eigenvalue is computed
  - Not very accurate
  - Copies of this eigenvalue
  - Small error of recurrence relation
  - Large condition numbers of Hessenberg matrices in RKS

  For this problem, constant continuation vector works fine for $k \leq 10$.
- Continue with last Krylov vector (20 iterations)

λ	$\|B_N^{-1}A_N x - \lambda x\|_2$	$\|A(\lambda)x\|_2$
8.127	$1.0 \cdot 10^{-12}$	$6.0 \cdot 10^{-12}$
8.127	$1.1 \cdot 10^{-11}$	$7.4 \cdot 10^{-11}$
7.405	$8.6 \cdot 10^{-11}$	$4.3 \cdot 10^{-10}$

- Finding more than three eigenvalues is not possible for this problem *with this method*

Implementation details

- Be careful with divided differences:
  - Do not use many poles
  - Use Hermite interpolation $\rightarrow$ repeated poles
  - Use analytical computation of divided differences if possible
  - Advantage of Hermite interpolation: reuse of LU-factorization of $A - \sigma_j B$.
- Exploit low rank structure:
  - The storage cost for k iterations is

$$n + (n+n) + (n+n+n) + \cdots + \underbrace{n + \cdots + n}_{k+1\times} = \frac{(k+2)(k+1)}{2} n$$

  - If the nonlinear part is described by a matrix of rank $r \ll n$:

$$A - \lambda A_0 + F E(\lambda) G^T$$

with F and $G \in \mathbb{R}^{n\times r}$ and $E \in \mathbb{R}^{r\times r}$. Storage cost:

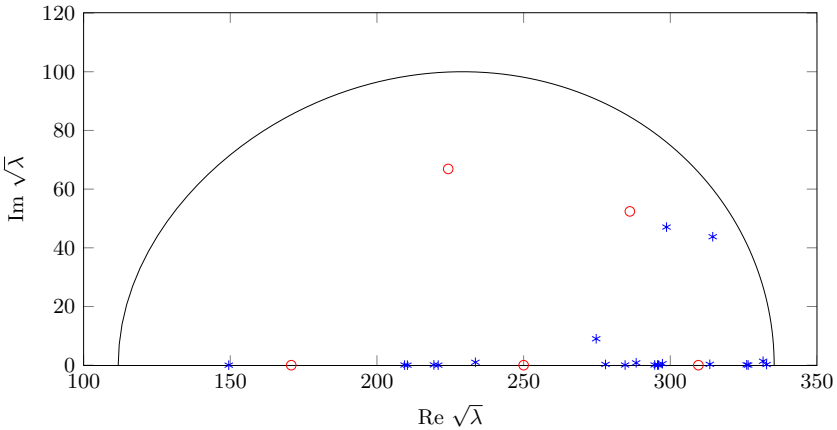
$$n + (n+n) + (n+n+r) + \cdots + n + n + \underbrace{r + \cdots + r}_{k-1\times} = \frac{k(k-1)}{2} r + 2nk$$

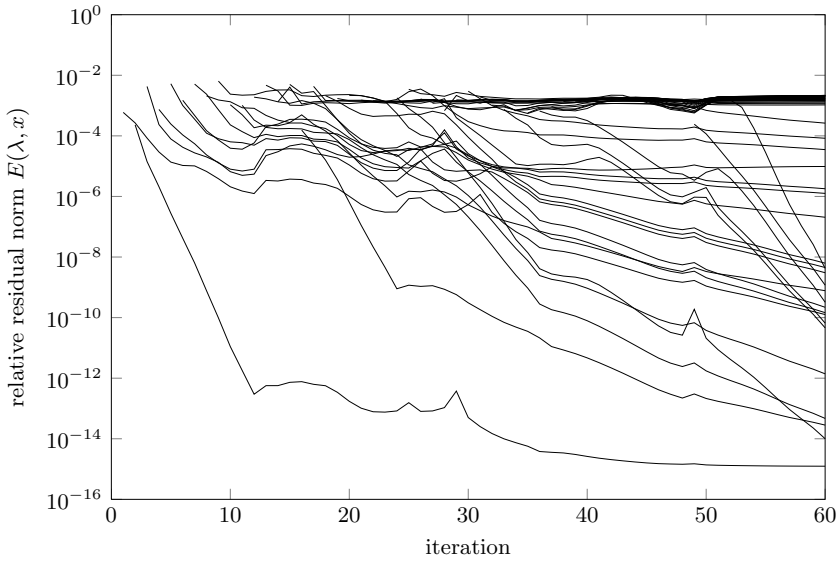
Gun problem

- Problem from the NLEVP collection

$$(K - \lambda M + i\sqrt{\lambda - \sigma_1^2}W_1 + i\sqrt{\lambda - \sigma_2^2}W_2)x = 0$$

  where K has order 9956 and $\text{rank}(W_1) + \text{rank}(W_2) = 84$.
- The goal is to compute all eigenvalues in a halve circle in the λ-plane
- We chose five interpolation points equally distributed in the λ-plane





Gun problem

- Impact of exploitation of low rank in the nonlinearity:

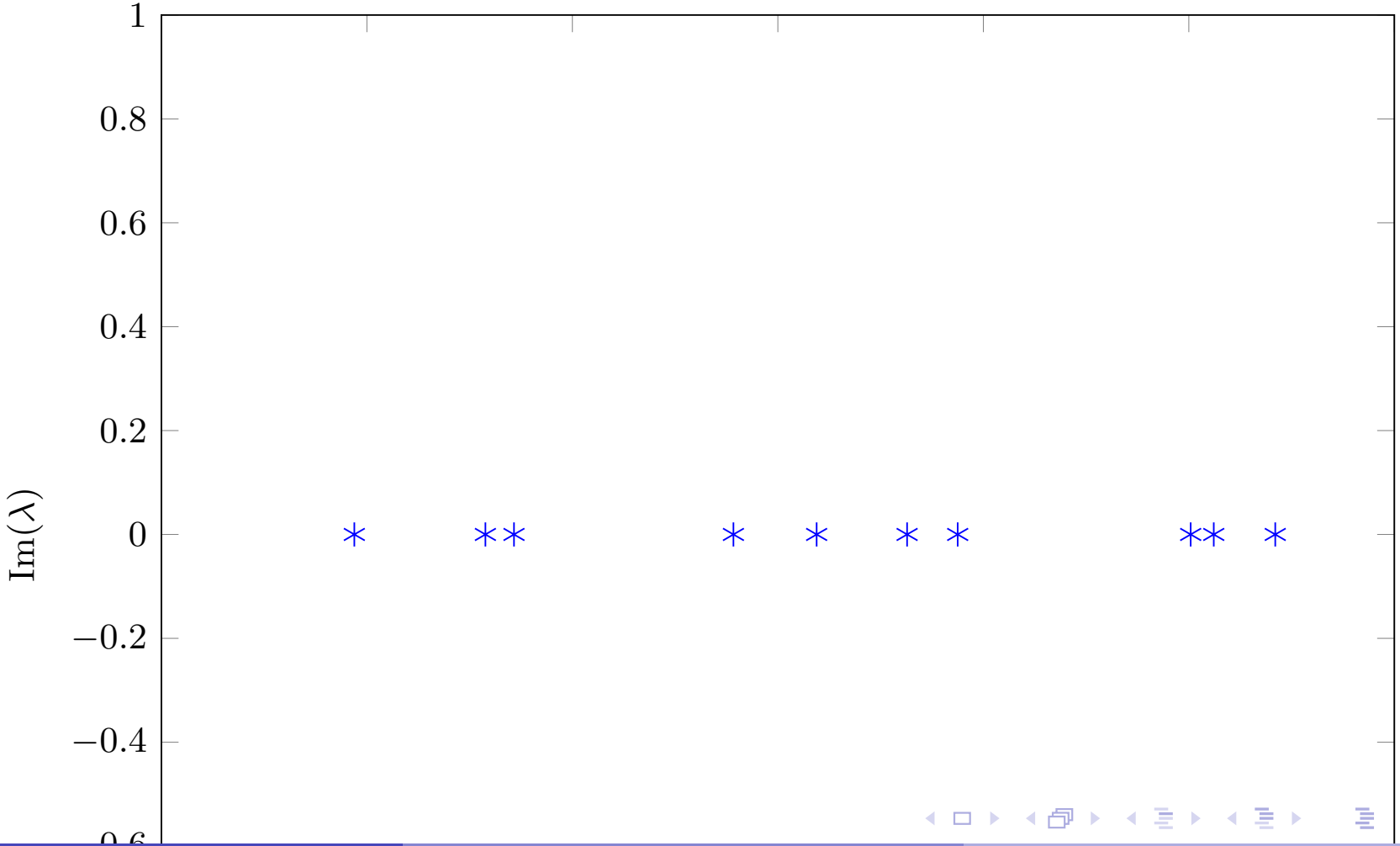
	RKS	RKS + rank reduction
LU decompositions	5.3s	5.3s
Linear system solves	2.4s	2.4s
Gram-Schmidt orth. + reorth.	29.7s	1.2s
Total	40.7s	8.9s

Schrödinger equation

- 2D equation

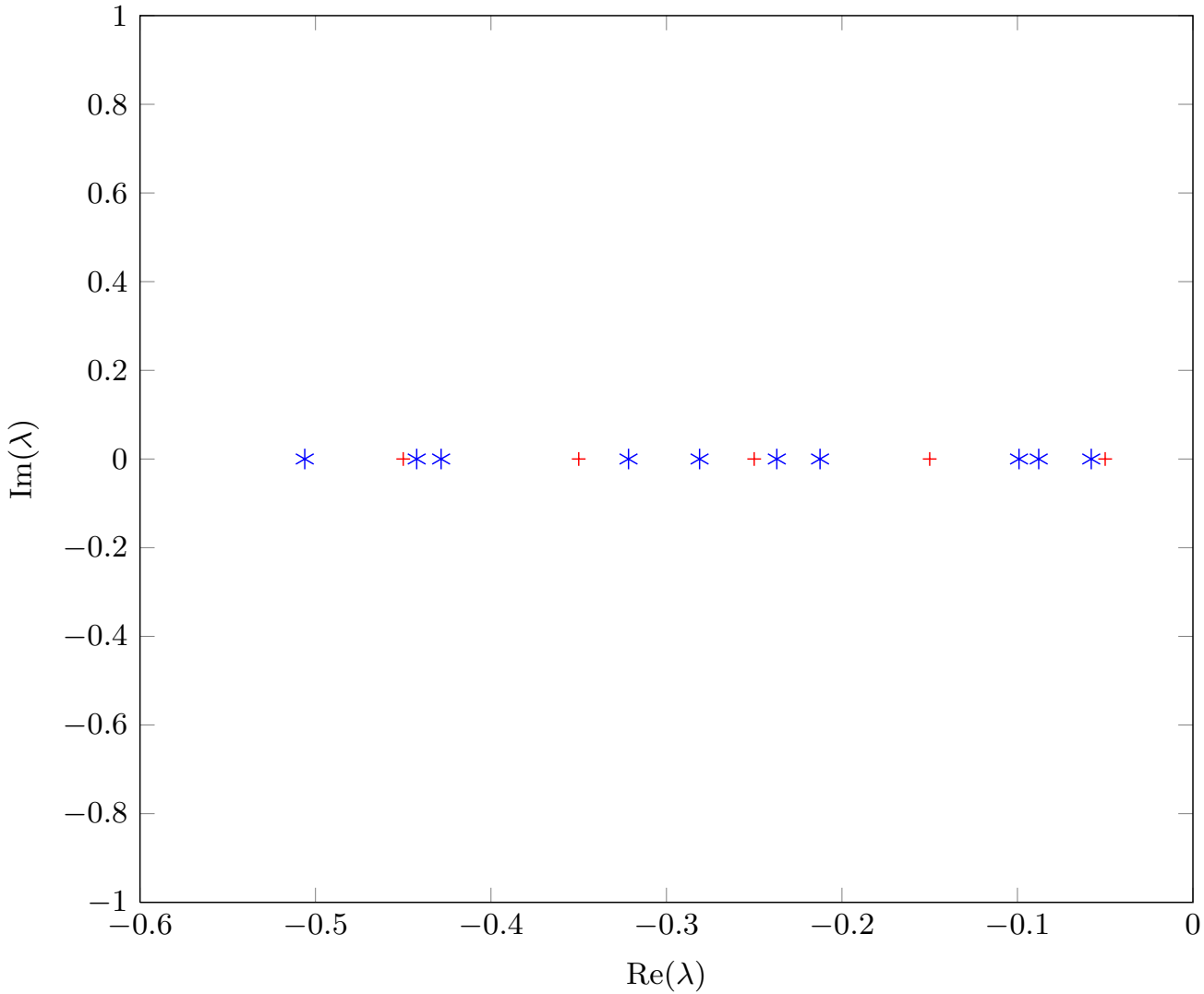
$$(H + E_2 \exp(-i\sqrt{\lambda - D})E_2^T)x = \lambda x$$

E_2 is rank $\sqrt{n}$ matrix, D is diagonal.



2D Schrödinger equation

- Overview convergence:
  - 25 iterations with $\sigma = 0.05, 0.15, 0.25, 0.35, 0.45$



Conclusions

- More numerical experiments needed, for other problems
- Advantages of rational Krylov:
  - Low degree polynomials
  - With or without derivatives
  - Exploit structure, use symbolic tools
- Disadvantages of rational Krylov:
  - Works well on most problems tried out when using Hermite interpolation
  - Newton polynomials require divided differences
- Overall conclusion:
  - Poles chosen for interpolation (see Olmstead, sqrt, exp): be careful
  - Hermite interpolation with symbolic tool works well