Rational Krylov methods for linear and nonlinear eigenvalue problems

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20 March 2014

Outline

- Shift–invert Arnoldi algorithm for linear eigenproblems
- Rational Krylov algorithm for linear eigenproblems
- Applications of Rational Krylov algorithm for nonlinear eigenproblems
  - Linearization by means of Hermite interpolation
  - Nonlinear Rational Krylov

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Linear eigenvalue problem

Definition of the problem

Given $A, B \in \mathbb{C}^{n \times n}$ find pairs $(\lambda, x) \in \mathbb{C} \times \mathbb{C}^n$ such that

$$Ax = \lambda Bx$$

The number λ is called eigenvalue
The vector x is called eigenvector

In practical applications:

- matrices are big sized, sparse and/or structured and/or (reducible to) small bandwidth etc.
- the task is to compute a well defined subset of eigenvalues, e.g. dominant eigenvalues, eigenvalue in a subset $\Omega \subset \mathbb{C}$ etc.

Shift–invert Arnoldi algorithm

Chosen a point (called shift) $\sigma \in \mathbb{C}$, this algorithm compute eigenvalues near σ.

Observation

If (θ, x) is an eigenpair of $(A - \sigma B)^{-1}B$, then $(\sigma + 1/\theta, x)$ is an eigenpair of the pencil (A, B).

Definition (Krylov subspace)

Given a vector $x \in \mathbb{C}^n$, a shift $\sigma \in \mathbb{C}$ and a natural number m

$$K_m(A, B, \sigma, x) = \text{span}\left(x, (A - \sigma B)^{-1}Bx, (A - \sigma B)^{-2}B^2x, \ldots, (A - \sigma B)^{-m+1}B^{m-1}x\right)$$

is the Krylov subspace

The idea is to project the matrix $(A - \sigma B)^{-1}B$ in the Krylov subspace and solve the projected problem.

Shift–invert Arnoldi algorithm

Gram–Schmidt orthogonalization

Given $x \in \mathbb{C}^n$ define

$$\begin{cases} v_1 := x/\|x\| & \\ h_{i,j} = (A - \sigma B)^{-1} B v_j \cdot v_i & i = 1, \dots j \\ w_{j+1} := (A - \sigma B)^{-1} B v_j - h_{1,j} v_1 - h_{2,j} v_2 - \cdots - h_{j,j} v_j & \\ h_{j+1,j} = \|w_{j+1}\| & \\ v_{j+1} = w_{j+1}/h_{j+1,j} & \end{cases}$$

Then $v_1, \dots, v_m$ is an orthonormal basis of $K_m(A, \sigma, x)$.

Arnoldi sequence

In a vectorial form

$$(A - \sigma B)^{-1} B V_m = V_{m+1} H_{m+1,m}$$

Shift–invert Arnoldi algorithm

Observation

The matrix $H_{m,m}$ is the projection of $(A-\sigma B)^{-1}B$ in $K_m(A,\sigma,x)$, that is

$$V_m^H(A-\sigma B)^{-1}BV_m = H_{m,m}$$

Definition

Given an eigenpair (θ, s) of $H_{m,m}$, the value $\lambda := \sigma + 1/\theta$ is called Ritz value and the vector $z := V_m s$ Ritz vector.

Proposition

If (θ, s) is an eigenpair of $H_{m,m}$ then

$$Az - \lambda Bz = \left(\frac{\sigma B - A}{\theta}\right) h_{m+1,m} s_m v_{m+1}.$$

If $h_{m+1,m}y_m$ is small, then $(\theta, V_m s)$ is an approximation of an eigenpair of the the linear problem defined by A and B.

Shift–invert Arnoldi algorithm

Algorithm

1: Chose a starting vector x and a shift σ
2: **for** $m = 1, \ldots,$ till convergence **do**
3: Compute the Arnoldi sequence $(A - \sigma B)^{-1} B V_m = V_{m+1} H_{m+1,m}$
4: Compute eigenpairs (θ_i, y_i) of $H_{m,m}$
5: **if** $|h_{m+1,m}(e_m^H y_i)| < tol$ **then**
6: Store $(\sigma + 1/\theta_i, V_m y_i)$ as approximation of an eigenpair of (A, B)
7: **end if**
8: **end for**

Questions:

- How big must be m to get a good approximation of an eigenpair?
- How to choose a starting vector x?
- Which eigenpairs will be firstly approximated?

Shift–invert Arnoldi algorithm

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Convergence of the algorithm

- Eigenvalues near σ will be firstly well approximate by Ritz values [Saad].
- The closer (σ, x) to the eigenpair (λ, u) the faster the convergence to (λ, u) [Saad].
- For many applications, after a few steps, Ritz values converges linearly to eigenvalues.

Thick restart

Problem

When the Arnoldi sequence grows too long, every step of the Arnoldi iteration gets slower. Moreover orthogonality is numerically lost.

Thick restart

Let $(A-\sigma B)^{-1}BV_m = V_{m+1}H_{m+1,m}$ be an Arnoldi sequence with $\lambda_1, \ldots, \lambda_k$ a subset of Ritz values, where at least one has not converged yet. Then it is possible to build another Arnoldi sequence $(A-\sigma B)^{-1}BW_k = W_{k+1}\widetilde{H}_{k+1,k}$ such that $\lambda_1, \ldots, \lambda_k$ are the Ritz values.

The generation of the new sequence is numerically stable since it is done using Householder transformations.

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Shift–invert Arnoldi algorithm for the linear eigenproblem

Task: compute eigenvalues of the pair (A, B) in Ω.

- Select (enough) shifts: $\sigma_0, \ldots, \sigma_t \in \Omega$,
- use shift–invert Arnoldi's algorithm for every shift.

Problem

Every time we change shift we need to restart the algorithm.

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Rational Krylov algorithm for linear eigenvalue problem

Theorem (Ruhe)

In $O(m^3)$ it is possible change shift in the Arnoldi sequence, in particular

$$(A - \sigma_0 B)^{-1} B V_m = V_{m+1} H_{m+1,m} \Longrightarrow (A - \sigma_1 B)^{-1} B W_m = W_{m+1} \widetilde{H}_{m+1,m}$$

moreover $\text{span}(V_{m+1}) = \text{span}(W_{m+1})$. These operations are numerically stable if σ_0 and σ_1 are far enough from the eigenvalues of the original problem.

Rational Krylov algorithm for linear eigenvalue problem

Rational Krylov algorithm

1: Chose a starting vector x and a starting shift σ_0 and define $v_1 = x/\|x\|$.
2: **for** $i = 1, \ldots,$ till convergence **do**
3: Extend the Arnoldi sequence $(A - \sigma_i B)^{-1} B V_m = V_{m+1} H_{m+1,m}$ till enough Ritz values near σ_i numerically converge. When needed, perform a thick restart.
4: Chose the next shift σ_{i+1} and transform the previous Arnoldi sequence in $(A - \sigma_{i+1} B)^{-1} B V_m = V_{m+1} H_{m+1,m}$ ny using $O(m^3)$ ops.
5: **end for**

Practical issues

- When shift changes, an LU factorization of $(A - \sigma_{i+1} B)$ is performed
- Heuristically, a good choice of the next shift is taking the average of *cstep* (small) Ritz values not yet converged and near the previous shift.
- Thick restart is performed.

Rational Krylov algorithm for linear eigenvalue problem

Rational Krylov algorithm

1: Chose a starting vector x and a starting shift σ_0 and define $v_1 = x/\|x\|$.
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Numerical experimentation

Tubolar reactor model

The conservation of reactant and energy in a homogeneous tube of length L in dimensionless form is modeled by

$$\begin{cases} \dfrac{L}{v}\dfrac{dy}{dt} &= -\dfrac{1}{Pe_m}\dfrac{\partial^2 y}{\partial X^2} + \dfrac{\partial y}{\partial X} + Dye^{\gamma-\gamma T^{-1}}, \\ \dfrac{L}{v}\dfrac{dT}{dt} &= -\dfrac{1}{Pe_h}\dfrac{\partial^2 T}{\partial X^2} + \dfrac{\partial T}{\partial X} + \beta(T-T_0) - BDye^{\gamma-\gamma T^{-1}}, \end{cases}$$

$$\text{B.C. :} \qquad y'(0) = Pe_m y(0),\ T'(0) = Pe_h T(0),\ y'(1) = 0,\ T'(1) = 0.$$

Where y is the concentration, T the temperature and $0 \leq X \leq 1$ the spatial coordinate. The setting of the problem is
$Pe_m = Pe_h = 5, B = 0.5, \gamma = 25, \beta = 3,5, D = 0,2662$ and $L/v = 1$.

The task is to solve numerically the equation with the method of lines.

Numerical experimentation

Stability of the time discretization

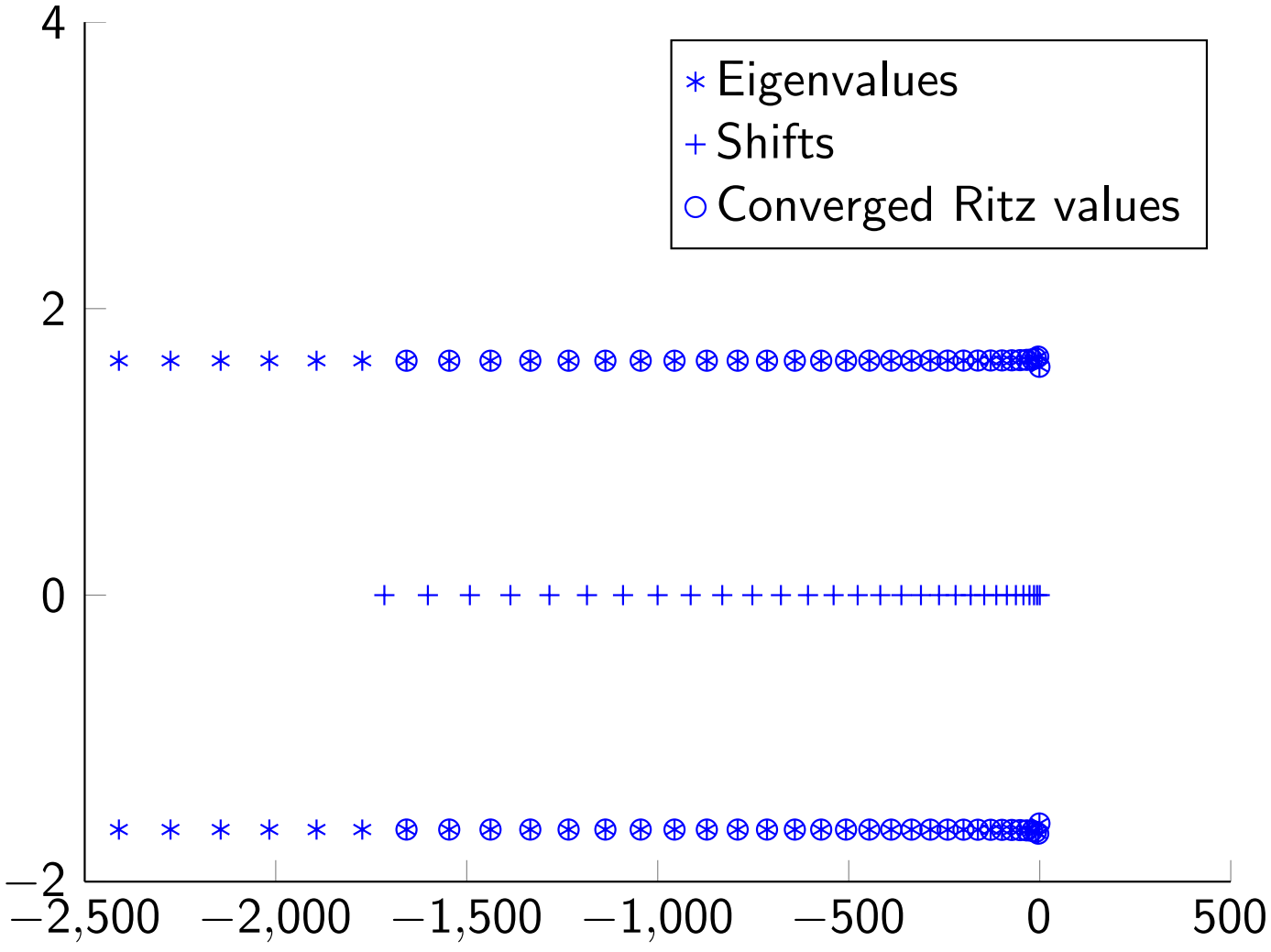
With a semi-discretization in space, setting $x = (y_1, T1, y_2, T_2, \ldots, y_{N/2}, T_{N/2})$ we get

$$\frac{d}{dt}\mathbf{x} = Ax \qquad A \in \mathbb{R}^{2N \times 2N},$$

where $h = 1/N$ is the discretization step. A is a banded matrix with bandwidth 5. In order to chose a stable time discretization it is needed to compute the rightmost eigenvalues of A.

Numerical experimentation

$N = 500$, Rational Krylov algorithm to compute 60 rightmost eigenvalues

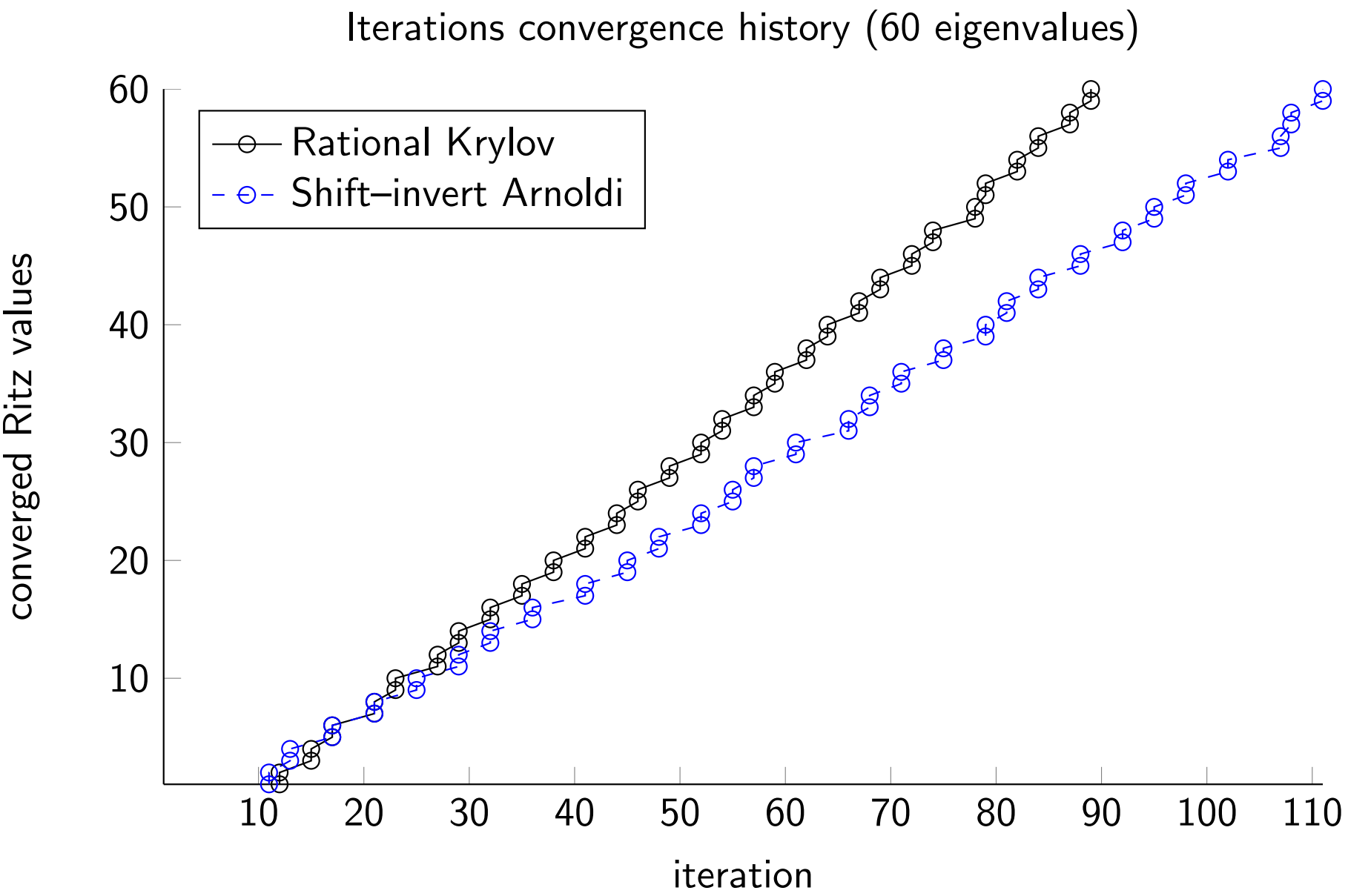


Numerical experimentation

Convergence of the rightmost eigenvalues with shift–invert Arnoldi and with Rational Krylov

Wanted eigenvalues	Shift–invert (number of steps)	Rational Krylov (number of steps)	Savings percentage (steps)
20	45	38	16 %
40	79	64	19 %
60	112	89	21 %
80	144	113	22 %

Numerical experimentation



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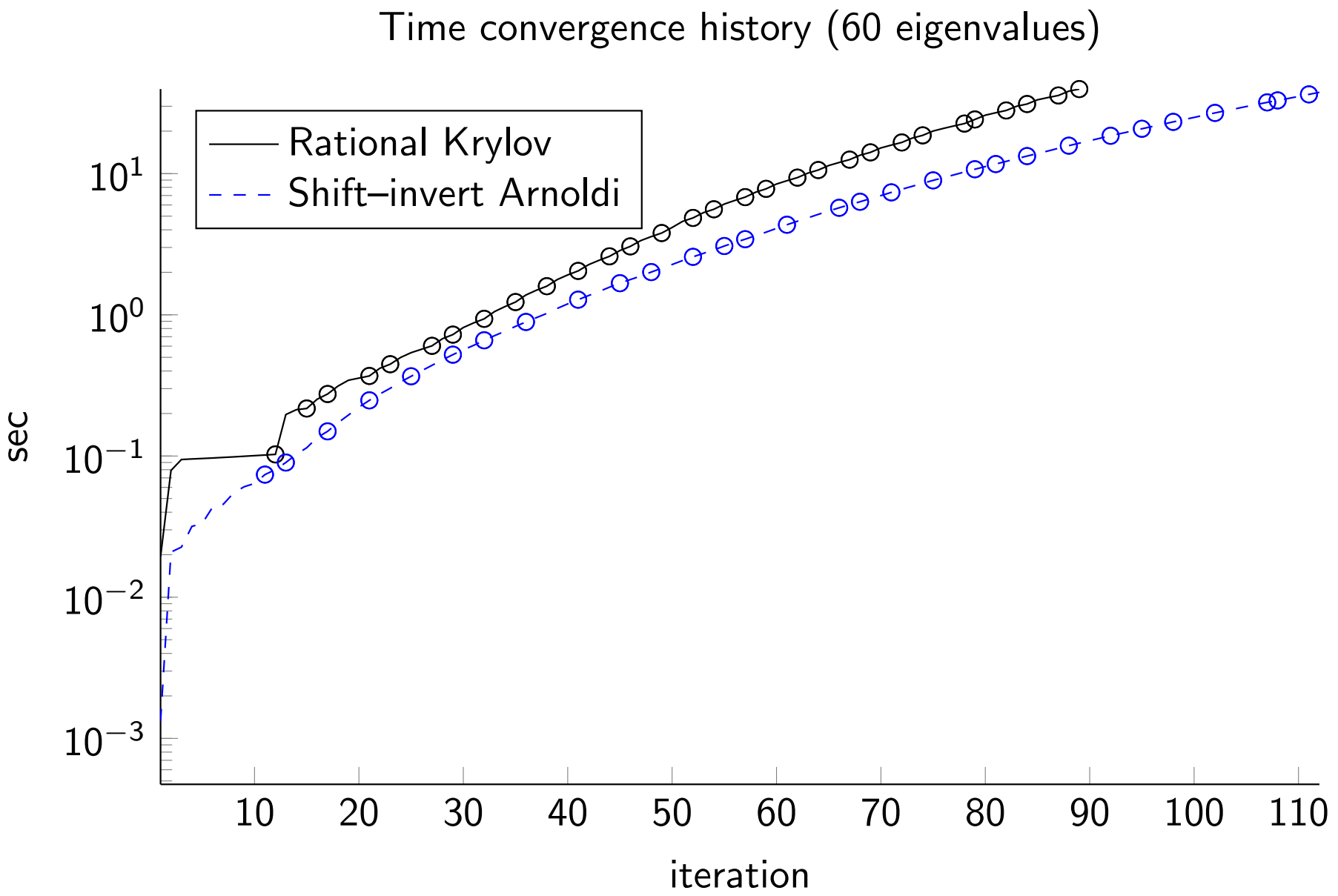


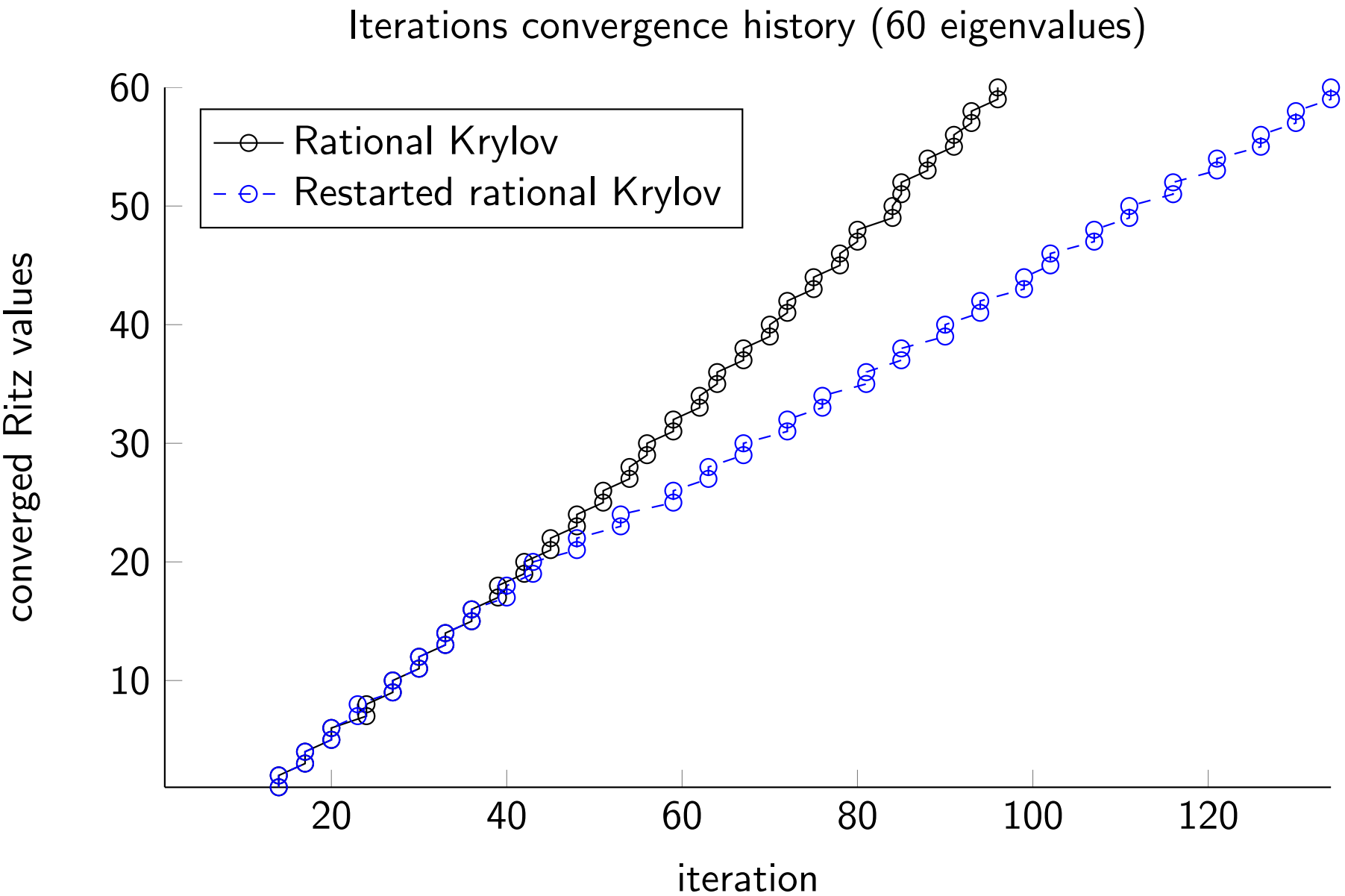
Numerical experimentation

With Rational Krylov it is possible to perform a thick restart. With shift–invert Arnoldi, if we do not lock all converged Ritz values, there is a loop.

We restart the Arnoldi sequence when the length is more than 40 and we lock the 20 Ritz values near the current shift.

This restarting strategy is not possible with shift–invert Arnoldi.

Numerical experimentation



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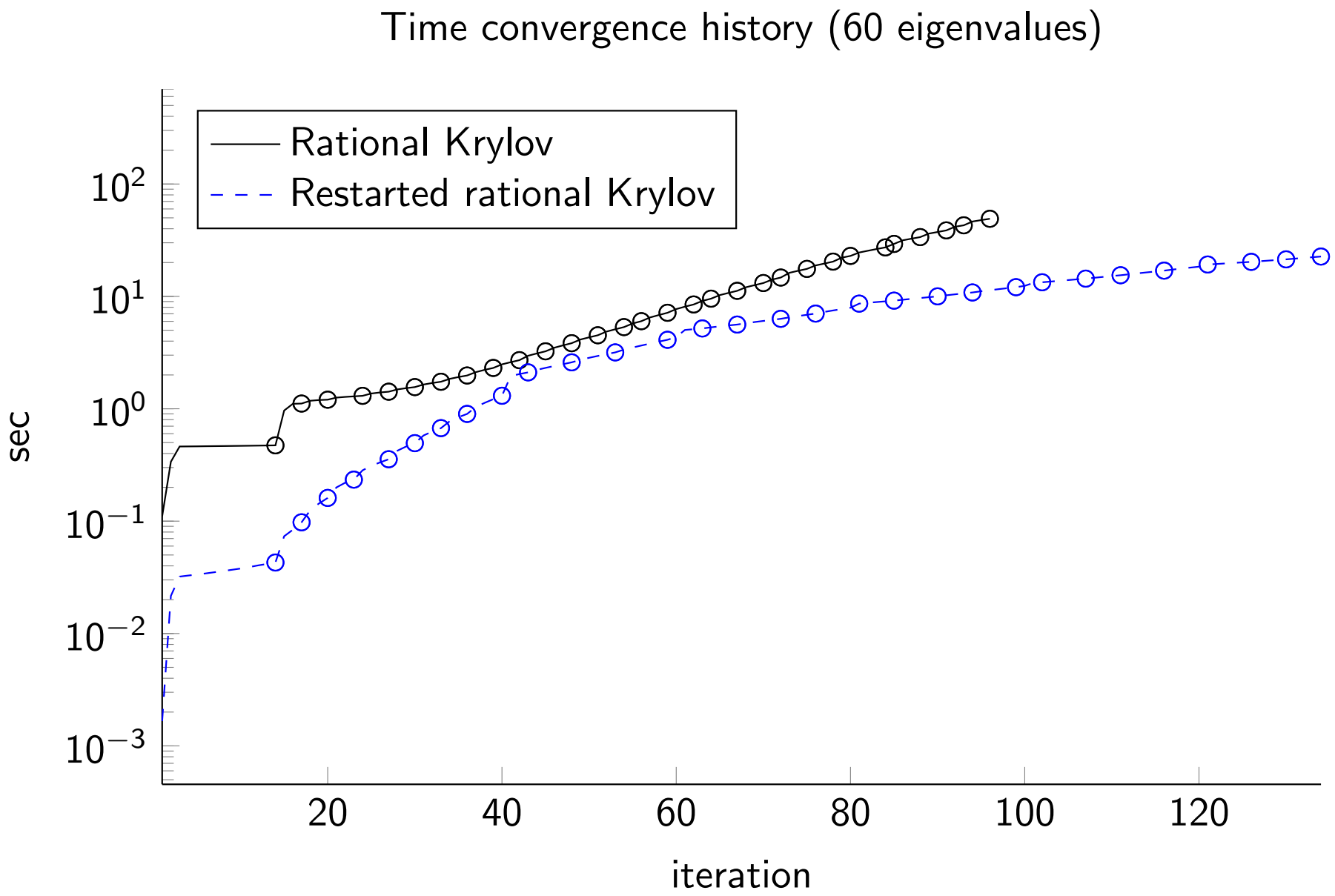

Numerical experimentation

Stability of a flow in a pipe

$$\begin{cases} \left\{(D^2-\alpha)^2 - i\alpha Re[\mathcal{U}_0(D^2-\alpha^2) - \mathcal{U}_0'']\right\}\tilde{v} = -ic\alpha Re(D^2-\alpha^2)\tilde{v} \\ \tilde{v}(1) = 0, \qquad D\tilde{v}(1)y = 0 \\ \tilde{v}(-1) = 0, \qquad D\tilde{v}(-1) = 0 \end{cases}$$

The setting is $\alpha = 1$ and $Re = 10000$.

Discrete problem

Using finite differences, we discretized with discretization step $h = 1/N$

$$A\underline{\tilde{v}} = cB\underline{\tilde{v}}$$

Where $A, B \in \mathbb{R}^{N\times N}$, $\det(A) \neq 0$, $\operatorname{rank}(B) = N - 4$ because of B.C.
A and B are banded matrices with bandwidth respectively 5 and 3.

The spectrum of the continuum problem has a branch structure, in particular it looks like a Y. The task is to compute the branch connected to zero.

Numerical experimentation

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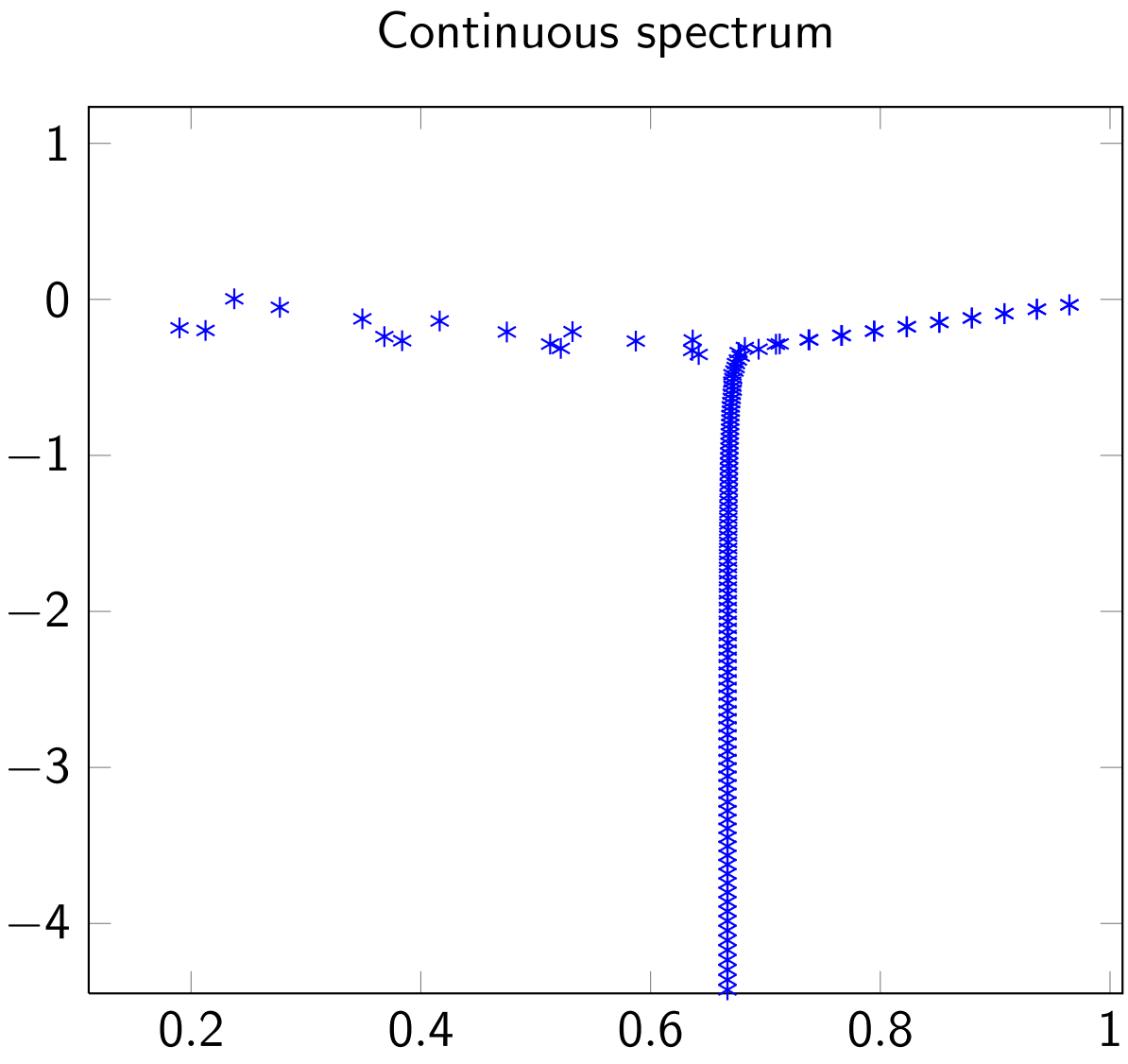
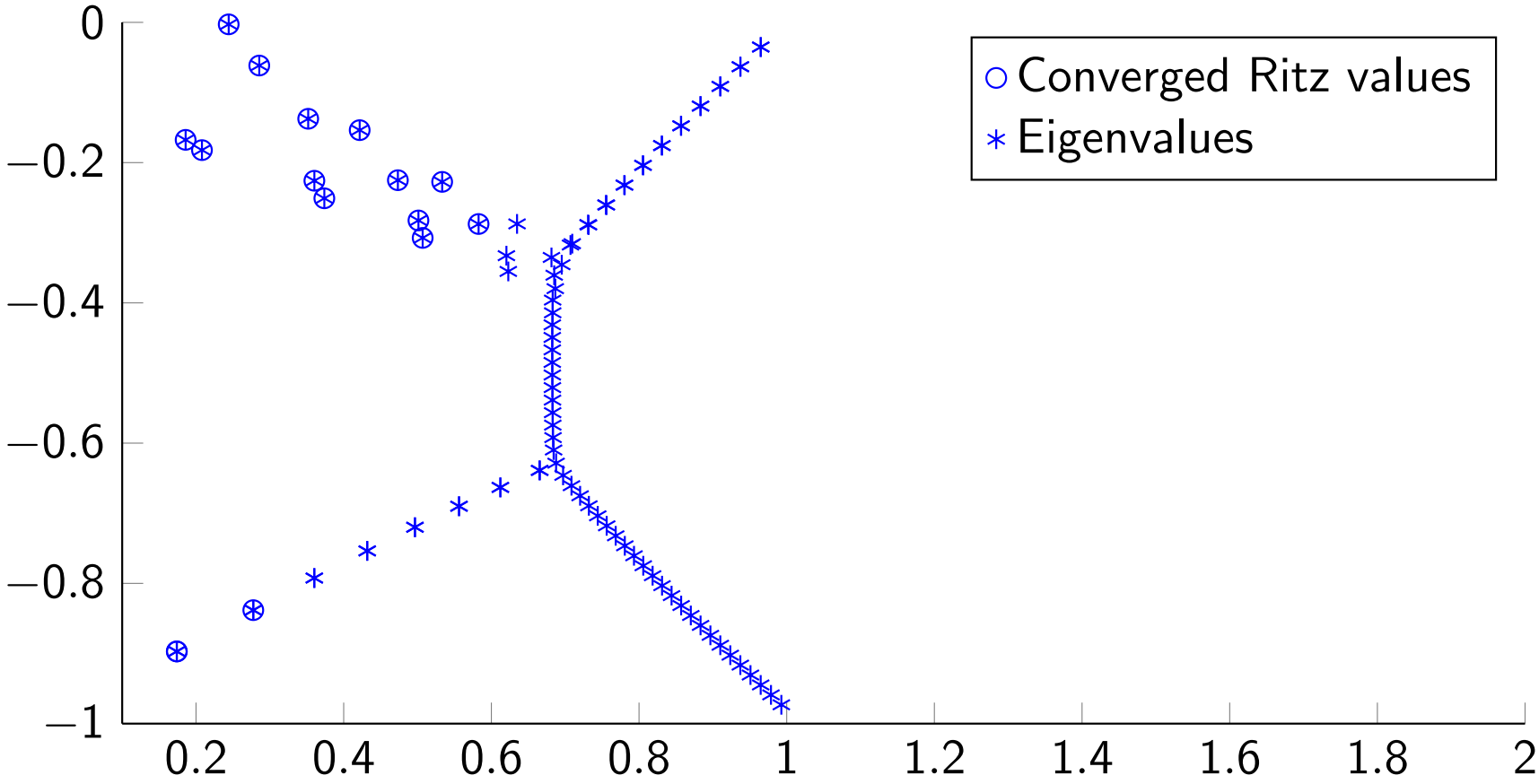


Numerical experimentation

$N = 100$, Ritz values computed with shift–invert Arnoldi.



Numerical experimentation

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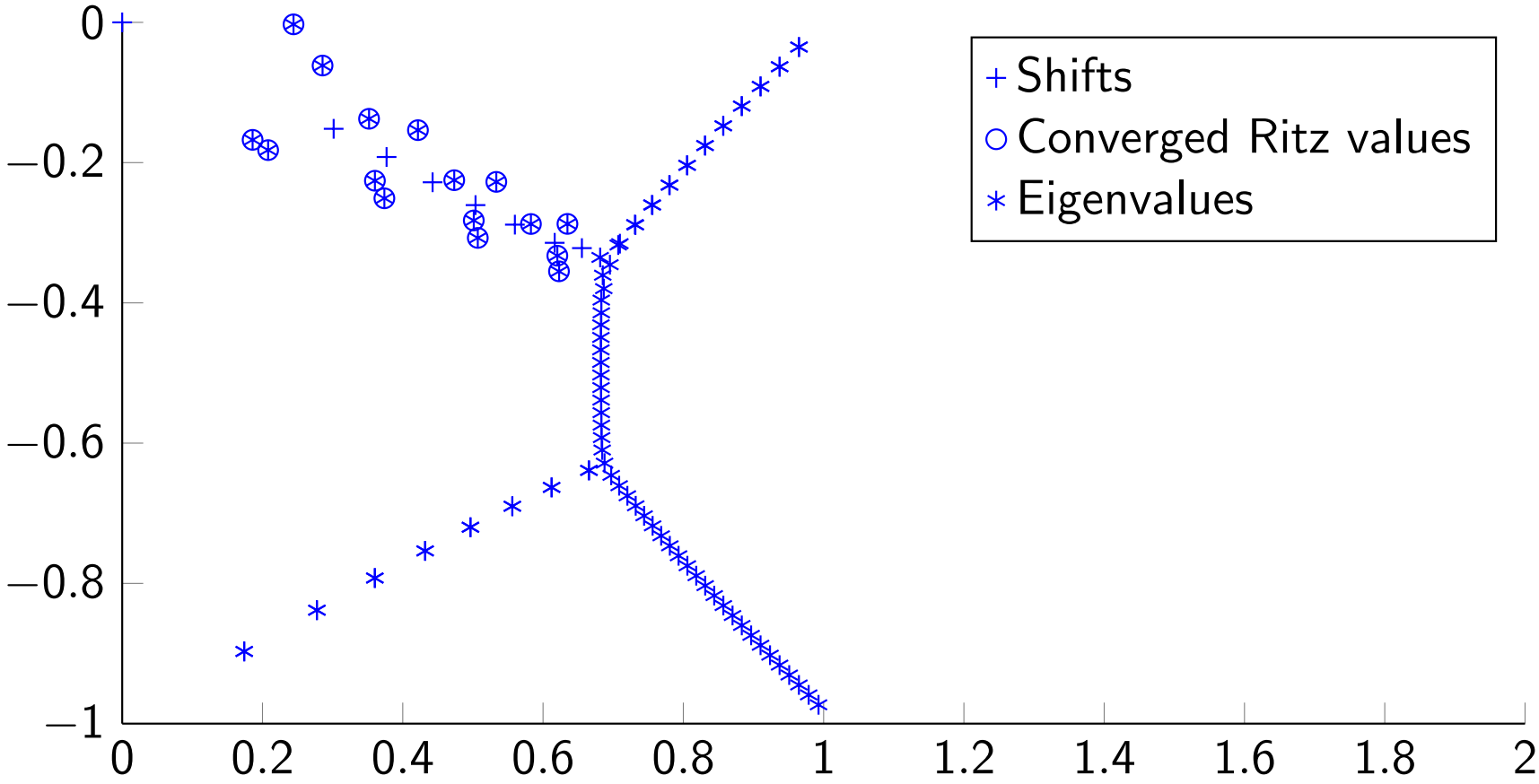

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Nonlinear eigenvalue problem and linearization

Nonlinear eigenvalue problem (NLEP)

Given a nonlinear application

$$A(\cdot) : \mathbb{C} \to \mathbb{C}^{n \times n}$$

the task is to compute $(\lambda, x) \in \mathbb{C} \times \mathbb{C}^n$ such that $A(\lambda)x = 0$ with $\lambda \in \Omega \subset \mathbb{C}$

Linearization

Given a nonlinear eigenvalue problem, a linearization is a linear eigenvalue problem such that its eigenpairs in Ω are a good estimation of eigeinpairs in Ω of the nonlinear problem.

We can every time express the nonlinear eigenvalue problem as

$$A(\lambda) = \sum_{i=1}^{m} f_i(\lambda) B_i \qquad \begin{array}{l} B_i \in \mathbb{C}^{n \times n} \\ f_i : \mathbb{C} \to \mathbb{C} \end{array}$$

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Linearization by means of Hermite interpolation

Consider the NLEP defined by

$$A(\lambda) = \sum_{i=1}^{m} f_i(\lambda) B_i$$

and select a set of points $\sigma_0, \ldots, \sigma_N \in \Omega$ (repetitions are allowed)

$$f_j(\lambda) \xrightarrow[\text{interpolation}]{\text{Hermite}} \sum_{i=0}^{N} \alpha_{i,j} n_i(\lambda)$$

then we can approximate the NLEP with a PEP defined by

$$P_N(\lambda) = \sum_{i=0}^{N} n_i(\lambda) A_i \qquad \text{where} \qquad A_i = \sum_{j=1}^{m} \alpha_{i,j} B_j$$

Linearization by means of Hermite interpolation

Theorem (Companion-type linearization)

The pair $(\lambda, x) \neq 0$ is an eigenpair of the PEP if and only if $\mathcal{A}_N y_N = \lambda \mathcal{B}_N y_N$ where

$$\mathcal{A}_N := \begin{pmatrix} A_0 & A_1 & A_2 & \dots & A_N \\ \sigma_0 I & I & & & \\ & \sigma_1 I & I & & \\ & & \ddots & \ddots & \\ & & & \sigma_{N-1} I & I \end{pmatrix}, \mathcal{B}_N := \begin{pmatrix} 0 & & & & \\ I & 0 & & & \\ & I & 0 & & \\ & & \ddots & \ddots & \\ & & & I & 0 \end{pmatrix}, y_N := \begin{pmatrix} x \\ n_1(\lambda)x \\ n_2(\lambda)x \\ n_3(\lambda)x \\ \vdots \\ n_N(\lambda)x \end{pmatrix}$$

Advantages

- Since $A_i = \sum_{j=1}^{m} \alpha_{i,j} B_j$, it is not needed to store A_i, it is sufficient to store the interpolation coefficients $\alpha_{i,j}$.
- If it is needed to add an interpolation point, we just need to one can just compute (implicitly) A_{N+1} and add a column and a row to the linearization matrices.
- Only the coefficients $\alpha_{i,j}$ are stored, all the other matrices are implicitly built.

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Rational Krylov algorithm to solve the linearized problem

Lemma

Consider the linear problem defined by the linearization $(\mathcal{A}_N, \mathcal{B}_N)$*, apply the rational Krylov algorithm by using as shifts the interpolation points and*

$$v_1 := vec\left(v_1^{[1]}, 0, \ldots, 0\right), \quad v_1 \in \mathbb{C}^{(N+1)n}, \quad v_1^{[1]} \in \mathbb{C}^n$$

as starting vector. Then at the j*-th step of the rational Krylov algorithm the vectors of the Arnoldi sequence have the following structure*

$$v_k = vec\left(v_k^{[1]}, v_k^{[2]}, \ldots, v_k^{[j]}, 0, \ldots, 0\right), \quad for \quad k \leq j \leq N,$$

where $v_k^{[i]} \in \mathbb{C}^n$ *for* $i = 1, \ldots, j$.

Building the basis of the Krylov subspace

Size of linearization: $N = 8$ (blocks)
Nodes/shifts: σ_0 σ_0 σ_0 σ_1 σ_1 σ_2 σ_2

$$v_1 = \begin{pmatrix} v_1^{[1]} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

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$$v_2 = \begin{pmatrix} v_2^{[1]} & v_2^{[2]} & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

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Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2	
$v_1 = ($	$v_1^{[1]}$	0	0	0	0	0	0	0 $)$
$v_2 = ($	$v_2^{[1]}$	$v_2^{[2]}$	0	0	0	0	0	0 $)$
$v_3 = ($	$v_3^{[1]}$	$v_3^{[2]}$	$v_3^{[3]}$	0	0	0	0	0 $)$

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$$
\begin{aligned}
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v_3 &= \begin{pmatrix} v_3^{[1]} & v_3^{[2]} & v_3^{[3]} & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \\
v_4 &= \begin{pmatrix} v_4^{[1]} & v_4^{[2]} & v_4^{[3]} & v_4^{[4]} & 0 & 0 & 0 & 0 \end{pmatrix}
\end{aligned}
$$

Building the basis of Krylov subspace

Size of linearization: $N = 8$ (blocks)
Nodes/shifts: σ_0 σ_0 σ_0 σ_1 σ_1 σ_2 σ_2

$$
\begin{aligned}
w_1 &= (\; w_1^{[1]} \; w_1^{[2]} \; w_1^{[3]} \; w_1^{[4]} \; 0 \; 0 \; 0 \; 0 \;) \\
w_2 &= (\; w_2^{[1]} \; w_2^{[2]} \; w_2^{[3]} \; w_2^{[4]} \; 0 \; 0 \; 0 \; 0 \;) \\
w_3 &= (\; w_3^{[1]} \; w_3^{[2]} \; w_3^{[3]} \; w_3^{[4]} \; 0 \; 0 \; 0 \; 0 \;) \\
w_4 &= (\; w_4^{[1]} \; w_4^{[2]} \; w_4^{[3]} \; w_4^{[4]} \; 0 \; 0 \; 0 \; 0 \;)
\end{aligned}
$$

Building the basis of Krylov subspace

Size of linearization: $N = 8$ (blocks)

Nodes/shifts: σ_0 σ_0 σ_0 σ_1 σ_1 σ_2 σ_2

$$
\begin{aligned}
w_1 &= (\; w_1^{[1]} \; w_1^{[2]} \; w_1^{[3]} \; w_1^{[4]} \; 0 \; 0 \; 0 \; 0 \;) \\
w_2 &= (\; w_2^{[1]} \; w_2^{[2]} \; w_2^{[3]} \; w_2^{[4]} \; 0 \; 0 \; 0 \; 0 \;) \\
w_3 &= (\; w_3^{[1]} \; w_3^{[2]} \; w_3^{[3]} \; w_3^{[4]} \; 0 \; 0 \; 0 \; 0 \;) \\
w_4 &= (\; w_4^{[1]} \; w_4^{[2]} \; w_4^{[3]} \; w_4^{[4]} \; 0 \; 0 \; 0 \; 0 \;) \\
w_5 &= (\; w_5^{[1]} \; w_5^{[2]} \; w_5^{[3]} \; w_5^{[4]} \; w_5^{[5]} \; 0 \; 0 \; 0 \;)
\end{aligned}
$$

Building the basis of Krylov subspace

Size of linearization: $N = 8$ (blocks)

Nodes/shifts: σ_0 σ_0 σ_0 σ_1 σ_1 σ_2 σ_2

$$
\begin{aligned}
w_1 &= (\; w_1^{[1]} \; w_1^{[2]} \; w_1^{[3]} \; w_1^{[4]} \; 0 \; 0 \; 0 \; 0 \;) \\
w_2 &= (\; w_2^{[1]} \; w_2^{[2]} \; w_2^{[3]} \; w_2^{[4]} \; 0 \; 0 \; 0 \; 0 \;) \\
w_3 &= (\; w_3^{[1]} \; w_3^{[2]} \; w_3^{[3]} \; w_3^{[4]} \; 0 \; 0 \; 0 \; 0 \;) \\
w_4 &= (\; w_4^{[1]} \; w_4^{[2]} \; w_4^{[3]} \; w_4^{[4]} \; 0 \; 0 \; 0 \; 0 \;) \\
w_5 &= (\; w_5^{[1]} \; w_5^{[2]} \; w_5^{[3]} \; w_5^{[4]} \; w_5^{[5]} \; 0 \; 0 \; 0 \;) \\
w_6 &= (\; w_6^{[1]} \; w_6^{[2]} \; w_6^{[3]} \; w_6^{[4]} \; w_6^{[5]} \; w_6^{[6]} \; 0 \; 0 \;)
\end{aligned}
$$

Building the basis of Krylov subspace

Size of linearization: $N = 8$ (blocks)
Nodes/shifts: σ_0 σ_0 σ_0 σ_1 σ_1 σ_2 σ_2

$$
\begin{aligned}
z_1 &= (\; z_1^{[1]} \; z_1^{[2]} \; z_1^{[3]} \; z_1^{[4]} \; z_1^{[5]} \; z_1^{[6]} \; 0 \; 0 \;) \\
z_2 &= (\; z_2^{[1]} \; z_2^{[2]} \; z_2^{[3]} \; z_2^{[4]} \; z_2^{[5]} \; z_2^{[6]} \; 0 \; 0 \;) \\
z_3 &= (\; z_3^{[1]} \; z_3^{[2]} \; z_3^{[3]} \; z_3^{[4]} \; z_3^{[5]} \; z_3^{[6]} \; 0 \; 0 \;) \\
z_4 &= (\; z_4^{[1]} \; z_4^{[2]} \; z_4^{[3]} \; z_4^{[4]} \; z_4^{[5]} \; z_4^{[6]} \; 0 \; 0 \;) \\
z_5 &= (\; z_5^{[1]} \; z_5^{[2]} \; z_5^{[3]} \; z_5^{[4]} \; z_5^{[5]} \; z_5^{[6]} \; 0 \; 0 \;) \\
z_6 &= (\; z_6^{[1]} \; z_6^{[2]} \; z_6^{[3]} \; z_6^{[4]} \; z_6^{[5]} \; z_6^{[6]} \; 0 \; 0 \;)
\end{aligned}
$$

Building the basis of Krylov subspace

Size of linearization: $N = 8$ (blocks)

Nodes/shifts: σ_0 σ_0 σ_0 σ_1 σ_1 σ_2 σ_2

$$
\begin{aligned}
z_1 &= (\; z_1^{[1]} \; z_1^{[2]} \; z_1^{[3]} \; z_1^{[4]} \; z_1^{[5]} \; z_1^{[6]} \; 0 \; 0 \;) \\
z_2 &= (\; z_2^{[1]} \; z_2^{[2]} \; z_2^{[3]} \; z_2^{[4]} \; z_2^{[5]} \; z_2^{[6]} \; 0 \; 0 \;) \\
z_3 &= (\; z_3^{[1]} \; z_3^{[2]} \; z_3^{[3]} \; z_3^{[4]} \; z_3^{[5]} \; z_3^{[6]} \; 0 \; 0 \;) \\
z_4 &= (\; z_4^{[1]} \; z_4^{[2]} \; z_4^{[3]} \; z_4^{[4]} \; z_4^{[5]} \; z_4^{[6]} \; 0 \; 0 \;) \\
z_5 &= (\; z_5^{[1]} \; z_5^{[2]} \; z_5^{[3]} \; z_5^{[4]} \; z_5^{[5]} \; z_5^{[6]} \; 0 \; 0 \;) \\
z_6 &= (\; z_6^{[1]} \; z_6^{[2]} \; z_6^{[3]} \; z_6^{[4]} \; z_6^{[5]} \; z_6^{[6]} \; 0 \; 0 \;) \\
z_7 &= (\; z_7^{[1]} \; z_7^{[2]} \; z_7^{[3]} \; z_7^{[4]} \; z_7^{[5]} \; z_7^{[6]} \; z_7^{[7]} \; 0 \;)
\end{aligned}
$$

Building the basis of Krylov subspace

Size of linearization: $N = 8$ (blocks)

Nodes/shifts: σ_0 σ_0 σ_0 σ_1 σ_1 σ_2 σ_2

$$
\begin{aligned}
z_1 &= (\; z_1^{[1]} \; z_1^{[2]} \; z_1^{[3]} \; z_1^{[4]} \; z_1^{[5]} \; z_1^{[6]} \; 0 \; 0 \;) \\
z_2 &= (\; z_2^{[1]} \; z_2^{[2]} \; z_2^{[3]} \; z_2^{[4]} \; z_2^{[5]} \; z_2^{[6]} \; 0 \; 0 \;) \\
z_3 &= (\; z_3^{[1]} \; z_3^{[2]} \; z_3^{[3]} \; z_3^{[4]} \; z_3^{[5]} \; z_3^{[6]} \; 0 \; 0 \;) \\
z_4 &= (\; z_4^{[1]} \; z_4^{[2]} \; z_4^{[3]} \; z_4^{[4]} \; z_4^{[5]} \; z_4^{[6]} \; 0 \; 0 \;) \\
z_5 &= (\; z_5^{[1]} \; z_5^{[2]} \; z_5^{[3]} \; z_5^{[4]} \; z_5^{[5]} \; z_5^{[6]} \; 0 \; 0 \;) \\
z_6 &= (\; z_6^{[1]} \; z_6^{[2]} \; z_6^{[3]} \; z_6^{[4]} \; z_6^{[5]} \; z_6^{[6]} \; 0 \; 0 \;) \\
z_7 &= (\; z_7^{[1]} \; z_7^{[2]} \; z_7^{[3]} \; z_7^{[4]} \; z_7^{[5]} \; z_7^{[6]} \; z_7^{[7]} \; 0 \;) \\
z_8 &= (\; z_8^{[1]} \; z_8^{[2]} \; z_8^{[3]} \; z_8^{[4]} \; z_8^{[5]} \; z_8^{[6]} \; z_8^{[7]} \; z_8^{[8]} \;)
\end{aligned}
$$

Rational Krylov algorithm to solve the linearized problem

Lemma

At each iteration j of the rational Krylov algorithm, only the top-left parts of the matrices $\mathcal{A}_N - \sigma_j \mathcal{B}_N$ are used to compute the nonzero top parts $\tilde{v}_{j+1}$ of the vectors v_{j+1}, i.e.,

$$(\mathcal{A}_j - \sigma_j \mathcal{B}_j)\tilde{v}_{j+1} = \mathcal{B}_j \tilde{v}_j,$$

where

$$\tilde{v}_{j+1} = vec\left(v_{j+1}^{[1]}, v_{j+1}^{[2]}, \ldots, v_{j+1}^{[j+1]}\right),$$

and

$$\tilde{v}_j = vec\left(v_j^{[1]}, v_j^{[2]}, \ldots, v_j^{[j]}, 0\right),$$

Rational Krylov algorithm to solve the linearized problem

Lemma

The linear system $(\mathcal{A}_j - \sigma_j \mathcal{B}_j)\tilde{v}_{j+1} = \mathcal{B}_j \tilde{v}_j$ *can be efficiently solved by using the following equations*

$$A(\sigma_j) v_{j+1}^{[1]} = y_0^{(j)},$$

where

$$y_0^{(j)} = -\sum_{i=1}^{j} A_j \left(v_j^{[i]} + \sum_{k=1}^{i-1} \left(\prod_{l=k}^{i-1} \mu_l^{(j)} \right) v_j^{[k]} \right),$$

and

$$\begin{aligned} v_{j+1}^{[2]} &= v_j^{[1]} + \mu_0^{(j)} v_{j+1}^{[1]}, \\ v_{j+1}^{[3]} &= v_j^{[2]} + \mu_1^{(j)} v_{j+1}^{[2]}, \\ &\vdots, \\ v_{j+1}^{[j+1]} &= v_j^{[j]} + \mu_{j-1}^{(j)} v_{j+1}^{[j]}. \end{aligned}$$

HIRK (Hermite Interpolation Rational Krylov Method)

1: Choose the shift σ_0 and starting vector v_1.
2: **for** $j = 1, \ldots, m$ **do**
3: EXPANSION PHASE.
4: Choose the shift σ_j.
5: Compute the next divided difference: A_j.
6: Expand $\mathcal{A}_j$, $\mathcal{B}_j$ and V_j.
7: RATIONAL KRYLOV STEP
8: **if** $\sigma_{j-1} \neq \sigma_j$ **then**
9: Change basis $V_j \to \tilde{V}_j$ and matrix $H_{j,j-1} \to \tilde{H}_{j,j-1}$
(according to the Rational Krylov algorithm)
such that the Arnoldi sequence becomes

$$(\mathcal{A}_j - \sigma_j \mathcal{B}_j)^{-1} \mathcal{B}_j \tilde{V}_j = \tilde{H}_{j,j-1} V_{j-1}.$$

10: **end if**
11: Compute the next vector of the sequence:

$$r = (\mathcal{A}_j - \sigma_j \mathcal{B}_j)^{-1} \mathcal{B}_j v_j,$$

$$r = v - V_j h_j, \qquad \text{where} \quad h_j = V_j^H r \qquad \text{orthogonalization},$$

$$v_{j+1} = r / h_{j+1,j}, \qquad \text{where} \quad h_{j+1,j} = \|r\| \qquad \text{normalization}.$$

12: Compute the eigenpair (θ_i, y_i) for $i = 1, \ldots, j$ of $H_{j,j-1}$ and then the Ritz pairs $(\theta_i, V_j y_i)$.
13: Test the convergence for the NLEP.
14: **end for**

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts: σ_0 σ_0 σ_0 σ_1 σ_1 σ_2 σ_2

$v_1 = ($ $v_1^{[1]}$ $)$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts: σ_0 σ_0 σ_0 σ_1 σ_1 σ_2 σ_2

$v_1 = ($ $v_1^{[1]}$ 0 $)$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts: σ_0 σ_0 σ_0 σ_1 σ_1 σ_2 σ_2

$$v_1 = \begin{pmatrix} v_1^{[1]} & 0 \end{pmatrix}$$

$$v_2 = \begin{pmatrix} v_2^{[1]} & v_2^{[2]} \end{pmatrix}$$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts: σ_0 σ_0 σ_0 σ_1 σ_1 σ_2 σ_2

$$v_1 = \begin{pmatrix} v_1^{[1]} & 0 & 0 \end{pmatrix}$$

$$v_2 = \begin{pmatrix} v_2^{[1]} & v_2^{[2]} & 0 \end{pmatrix}$$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2

$$v_1 = \begin{pmatrix} v_1^{[1]} & 0 & 0 \end{pmatrix}$$

$$v_2 = \begin{pmatrix} v_2^{[1]} & v_2^{[2]} & 0 \end{pmatrix}$$

$$v_3 = \begin{pmatrix} v_3^{[1]} & v_3^{[2]} & v_3^{[3]} \end{pmatrix}$$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2

$$
\begin{aligned}
v_1 &= (\quad v_1^{[1]} \quad 0 \quad 0 \quad 0 \quad) \\
v_2 &= (\quad v_2^{[1]} \quad v_2^{[2]} \quad 0 \quad 0 \quad) \\
v_3 &= (\quad v_3^{[1]} \quad v_3^{[2]} \quad v_3^{[3]} \quad 0 \quad)
\end{aligned}
$$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2

$$
\begin{aligned}
v_1 &= (\quad v_1^{[1]} \quad 0 \quad 0 \quad 0 \quad) \\
v_2 &= (\quad v_2^{[1]} \quad v_2^{[2]} \quad 0 \quad 0 \quad) \\
v_3 &= (\quad v_3^{[1]} \quad v_3^{[2]} \quad v_3^{[3]} \quad 0 \quad) \\
v_4 &= (\quad v_4^{[1]} \quad v_4^{[2]} \quad v_4^{[3]} \quad v_4^{[4]} \quad)
\end{aligned}
$$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2

$$
\begin{aligned}
w_1 &= (\quad w_1^{[1]} \quad w_1^{[2]} \quad w_3^{[3]} \quad w_1^{[4]} \quad) \\
w_2 &= (\quad w_2^{[1]} \quad w_2^{[2]} \quad w_2^{[3]} \quad w_2^{[4]} \quad) \\
w_3 &= (\quad w_3^{[1]} \quad w_3^{[2]} \quad w_3^{[3]} \quad w_3^{[4]} \quad) \\
w_4 &= (\quad w_4^{[1]} \quad w_4^{[2]} \quad w_4^{[3]} \quad w_4^{[4]} \quad)
\end{aligned}
$$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2
$w_1 = ($	$w_1^{[1]}$	$w_1^{[2]}$	$w_3^{[3]}$	$w_1^{[4]}$	0	$)$	
$w_2 = ($	$w_2^{[1]}$	$w_2^{[2]}$	$w_2^{[3]}$	$w_2^{[4]}$	0	$)$	
$w_3 = ($	$w_3^{[1]}$	$w_3^{[2]}$	$w_3^{[3]}$	$w_3^{[4]}$	0	$)$	
$w_4 = ($	$w_4^{[1]}$	$w_4^{[2]}$	$w_4^{[3]}$	$w_4^{[4]}$	0	$)$	

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2

$$
\begin{aligned}
w_1 &= (\quad w_1^{[1]} \quad w_1^{[2]} \quad w_3^{[3]} \quad w_1^{[4]} \quad 0 \quad) \\
w_2 &= (\quad w_2^{[1]} \quad w_2^{[2]} \quad w_2^{[3]} \quad w_2^{[4]} \quad 0 \quad) \\
w_3 &= (\quad w_3^{[1]} \quad w_3^{[2]} \quad w_3^{[3]} \quad w_3^{[4]} \quad 0 \quad) \\
w_4 &= (\quad w_4^{[1]} \quad w_4^{[2]} \quad w_4^{[3]} \quad w_4^{[4]} \quad 0 \quad) \\
w_5 &= (\quad w_5^{[1]} \quad w_5^{[2]} \quad w_5^{[3]} \quad w_5^{[4]} \quad w_5^{[5]} \quad)
\end{aligned}
$$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2
$w_1 = ($	$w_1^{[1]}$	$w_1^{[2]}$	$w_3^{[3]}$	$w_1^{[4]}$	0	0	$)$
$w_2 = ($	$w_2^{[1]}$	$w_2^{[2]}$	$w_2^{[3]}$	$w_2^{[4]}$	0	0	$)$
$w_3 = ($	$w_3^{[1]}$	$w_3^{[2]}$	$w_3^{[3]}$	$w_3^{[4]}$	0	0	$)$
$w_4 = ($	$w_4^{[1]}$	$w_4^{[2]}$	$w_4^{[3]}$	$w_4^{[4]}$	0	0	$)$
$w_5 = ($	$w_5^{[1]}$	$w_5^{[2]}$	$w_5^{[3]}$	$w_5^{[4]}$	$w_5^{[5]}$	0	$)$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2
$w_1 = ($	$w_1^{[1]}$	$w_1^{[2]}$	$w_3^{[3]}$	$w_1^{[4]}$	0	0	$)$
$w_2 = ($	$w_2^{[1]}$	$w_2^{[2]}$	$w_2^{[3]}$	$w_2^{[4]}$	0	0	$)$
$w_3 = ($	$w_3^{[1]}$	$w_3^{[2]}$	$w_3^{[3]}$	$w_3^{[4]}$	0	0	$)$
$w_4 = ($	$w_4^{[1]}$	$w_4^{[2]}$	$w_4^{[3]}$	$w_4^{[4]}$	0	0	$)$
$w_5 = ($	$w_5^{[1]}$	$w_5^{[2]}$	$w_5^{[3]}$	$w_5^{[4]}$	$w_5^{[5]}$	0	$)$
$w_6 = ($	$w_6^{[1]}$	$w_6^{[2]}$	$w_6^{[3]}$	$w_6^{[4]}$	$w_6^{[5]}$	$w_6^{[6]}$	$)$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2
$z_1 = ($	$z_1^{[1]}$	$z_1^{[2]}$	$z_1^{[3]}$	$z_1^{[4]}$	$z_1^{[5]}$	$z_1^{[6]}$	$)$
$z_2 = ($	$z_2^{[1]}$	$z_2^{[2]}$	$z_2^{[3]}$	$z_2^{[4]}$	$z_2^{[5]}$	$z_2^{[6]}$	$)$
$z_3 = ($	$z_3^{[1]}$	$z_3^{[2]}$	$z_3^{[3]}$	$z_3^{[4]}$	$z_3^{[5]}$	$z_3^{[6]}$	$)$
$z_4 = ($	$z_4^{[1]}$	$z_4^{[2]}$	$z_4^{[3]}$	$z_4^{[4]}$	$z_4^{[5]}$	$z_4^{[6]}$	$)$
$z_5 = ($	$z_5^{[1]}$	$z_5^{[2]}$	$z_5^{[3]}$	$z_5^{[4]}$	$z_5^{[5]}$	$z_5^{[6]}$	$)$
$z_6 = ($	$z_6^{[1]}$	$z_6^{[2]}$	$z_6^{[3]}$	$z_6^{[4]}$	$z_6^{[5]}$	$z_6^{[6]}$	$)$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2
$z_1 = ($	$z_1^{[1]}$	$z_1^{[2]}$	$z_3^{[3]}$	$z_1^{[4]}$	$z_1^{[5]}$	$z_1^{[6]}$	0 $)$
$z_2 = ($	$z_2^{[1]}$	$z_2^{[2]}$	$z_2^{[3]}$	$z_2^{[4]}$	$z_2^{[5]}$	$z_2^{[6]}$	0 $)$
$z_3 = ($	$z_3^{[1]}$	$z_3^{[2]}$	$z_3^{[3]}$	$z_3^{[4]}$	$z_3^{[5]}$	$z_3^{[6]}$	0 $)$
$z_4 = ($	$z_4^{[1]}$	$z_4^{[2]}$	$z_4^{[3]}$	$z_4^{[4]}$	$z_4^{[5]}$	$z_4^{[6]}$	0 $)$
$z_5 = ($	$z_5^{[1]}$	$z_5^{[2]}$	$z_5^{[3]}$	$z_5^{[4]}$	$z_5^{[5]}$	$z_5^{[6]}$	0 $)$
$z_6 = ($	$z_6^{[1]}$	$z_6^{[2]}$	$z_6^{[3]}$	$z_6^{[4]}$	$z_6^{[5]}$	$z_6^{[6]}$	0 $)$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2
$z_1 = ($	$z_1^{[1]}$	$z_1^{[2]}$	$z_3^{[3]}$	$z_1^{[4]}$	$z_1^{[5]}$	$z_1^{[6]}$	0 $)$
$z_2 = ($	$z_2^{[1]}$	$z_2^{[2]}$	$z_2^{[3]}$	$z_2^{[4]}$	$z_2^{[5]}$	$z_2^{[6]}$	0 $)$
$z_3 = ($	$z_3^{[1]}$	$z_3^{[2]}$	$z_3^{[3]}$	$z_3^{[4]}$	$z_3^{[5]}$	$z_3^{[6]}$	0 $)$
$z_4 = ($	$z_4^{[1]}$	$z_4^{[2]}$	$z_4^{[3]}$	$z_4^{[4]}$	$z_4^{[5]}$	$z_4^{[6]}$	0 $)$
$z_5 = ($	$z_5^{[1]}$	$z_5^{[2]}$	$z_5^{[3]}$	$z_5^{[4]}$	$z_5^{[5]}$	$z_5^{[6]}$	0 $)$
$z_6 = ($	$z_6^{[1]}$	$z_6^{[2]}$	$z_6^{[3]}$	$z_6^{[4]}$	$z_6^{[5]}$	$z_6^{[6]}$	0 $)$
$z_7 = ($	$z_7^{[1]}$	$z_7^{[2]}$	$z_7^{[3]}$	$z_7^{[4]}$	$z_7^{[5]}$	$z_7^{[6]}$	$z_7^{[7]}$ $)$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2	
$z_1 = ($	$z_1^{[1]}$	$z_1^{[2]}$	$z_3^{[3]}$	$z_1^{[4]}$	$z_1^{[5]}$	$z_1^{[6]}$	0	0 $)$
$z_2 = ($	$z_2^{[1]}$	$z_2^{[2]}$	$z_2^{[3]}$	$z_2^{[4]}$	$z_2^{[5]}$	$z_2^{[6]}$	0	0 $)$
$z_3 = ($	$z_3^{[1]}$	$z_3^{[2]}$	$z_3^{[3]}$	$z_3^{[4]}$	$z_3^{[5]}$	$z_3^{[6]}$	0	0 $)$
$z_4 = ($	$z_4^{[1]}$	$z_4^{[2]}$	$z_4^{[3]}$	$z_4^{[4]}$	$z_4^{[5]}$	$z_4^{[6]}$	0	0 $)$
$z_5 = ($	$z_5^{[1]}$	$z_5^{[2]}$	$z_5^{[3]}$	$z_5^{[4]}$	$z_5^{[5]}$	$z_5^{[6]}$	0	0 $)$
$z_6 = ($	$z_6^{[1]}$	$z_6^{[2]}$	$z_6^{[3]}$	$z_6^{[4]}$	$z_6^{[5]}$	$z_6^{[6]}$	0	0 $)$
$z_7 = ($	$z_7^{[1]}$	$z_7^{[2]}$	$z_7^{[3]}$	$z_7^{[4]}$	$z_7^{[5]}$	$z_7^{[6]}$	$z_7^{[7]}$	0 $)$

Building the basis of Krylov subspace
Execution of the algorithm

Nodes/shifts:	σ_0	σ_0	σ_0	σ_1	σ_1	σ_2	σ_2	
$z_1 = ($	$z_1^{[1]}$	$z_1^{[2]}$	$z_3^{[3]}$	$z_1^{[4]}$	$z_1^{[5]}$	$z_1^{[6]}$	0	0 $)$
$z_2 = ($	$z_2^{[1]}$	$z_2^{[2]}$	$z_2^{[3]}$	$z_2^{[4]}$	$z_2^{[5]}$	$z_2^{[6]}$	0	0 $)$
$z_3 = ($	$z_3^{[1]}$	$z_3^{[2]}$	$z_3^{[3]}$	$z_3^{[4]}$	$z_3^{[5]}$	$z_3^{[6]}$	0	0 $)$
$z_4 = ($	$z_4^{[1]}$	$z_4^{[2]}$	$z_4^{[3]}$	$z_4^{[4]}$	$z_4^{[5]}$	$z_4^{[6]}$	0	0 $)$
$z_5 = ($	$z_5^{[1]}$	$z_5^{[2]}$	$z_5^{[3]}$	$z_5^{[4]}$	$z_5^{[5]}$	$z_5^{[6]}$	0	0 $)$
$z_6 = ($	$z_6^{[1]}$	$z_6^{[2]}$	$z_6^{[3]}$	$z_6^{[4]}$	$z_6^{[5]}$	$z_6^{[6]}$	0	0 $)$
$z_7 = ($	$z_7^{[1]}$	$z_7^{[2]}$	$z_7^{[3]}$	$z_7^{[4]}$	$z_7^{[5]}$	$z_7^{[6]}$	$z_7^{[7]}$	0 $)$
$z_8 = ($	$z_8^{[1]}$	$z_8^{[2]}$	$z_8^{[3]}$	$z_8^{[4]}$	$z_8^{[5]}$	$z_8^{[6]}$	$z_8^{[7]}$	$z_8^{[8]}$ $)$

Hermite Interpolation Rational Krylov Method

Comments

- At every step it is solved a system of the size of the original NLEP and not of the size of the linarization.
- The computation of the interpolation coefficients is numerically unstable. These coefficients must be computed semianalitically.
- Applying this method to a NLEP is like to solve a linear eigenvalue problem of infinite size.
- The bottleneck of the algorithm is the Gram–Schmidt process.
- At every step, the vectors of the basis of Krylov space get longer.
- Exploiting the low rank structure of the matrix coefficients can speedup the algorithm.

Outline

- Shift–invert Arnoldi algorithm for linear eigenproblems
- Rational Krylov algorithm for linear eigenproblems
- Applications of Rational Krylov algorithm for nonlinear eigenproblems
  - Linearization by means of Hermite interpolations
  - Nonlinear Rational Krylov

Nonlinear Rational Krylov

Definition (Generalized Arnoldi's sequence)

Given a pole $\sigma \in \Omega$ and a sequence of shifts $\lambda_1, \ldots, \lambda_m$ it holds

$$A(\sigma)^{-1} A(\lambda_m) V_m = V_{m+1} H_{m+1,m}$$

Generation of the sequence

$$A(\sigma)^{-1} A(\lambda_{j-1}) V_{j-1} = V_j H_{j,j-1} \xrightarrow[\text{interpolation}]{\text{linear}} A(\sigma)^{-1} A(\lambda_j) V_j = V_{j+1} \overline{H}_{j+1,j}.$$

Nonlinear Rational Krylov

Definition (Generalized Arnoldi's sequence)

Given a pole $\sigma \in \Omega$ and a sequence of shifts $\lambda_1, \ldots, \lambda_m$ it holds

$$A(\sigma)^{-1} A(\lambda_m) V_m = V_{m+1} H_{m+1,m}$$

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Nonlinear Rational Krylov

Observation

- With a linear Lagrange–interpolation between λ_j and σ we get the linearized problem

$$A(\lambda) = \frac{\lambda - \lambda_j}{\sigma - \lambda_j} A(\sigma) + \frac{\lambda - \sigma}{\lambda_j - \sigma} A(\lambda_j).$$

- If (θ, x) is such that

$$A(\sigma)^{-1} A(\lambda_j) x = \theta x$$

then (λ_{j+1}, x) is an eigenpair or the linearized problem, where

$$\lambda_{j+1} = \lambda_j + \frac{\theta}{1 - \theta}(\lambda_j - \sigma).$$

The closer θ to 0 the closer λ_{j+1} to λ_j.

Nonlinear Rational Krylov

Nonlinear Rational Krylov algorithm (Preliminary version)

1: Choose a starting vector v_1
2: **for** $j = 1, \ldots,$ till convergence **do**
3: Compute the Arnoldi sequence $A(\sigma)^{-1}A(\lambda_j)V_j = V_{j+1}H_{j+1,j}$
4: Compute the smallest eigenpairs (θ, s) of $H_{j,j}$
5: $\lambda_{j+1} = \lambda_j + \frac{\theta}{1-\theta}(\lambda_j - \sigma)$
6: $H_{j+1,j} = \frac{1}{1-\theta}H_{j+1,j} - \frac{\theta}{1-\theta}I_{j+1,j}$
7: **end for**

It turns out that this algorithm does not work well.

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Nonlinear Rational Krylov

Proposition

It holds

$$A(\sigma)^{-1}A(\lambda_{j+1})V_j - V_j H_{j,j} = A(\sigma)^{-1}A(\lambda_{j+1})V_j s\ e_j^H.$$

Observation

In the linear case it holds

$$A(\sigma)^{-1}A(\lambda_{j+1})V_j s = s_j h_{j+1,j} v_{j+1}$$

that is, the residual is orthogonal to V_m. This property does not hold in the nonlinear case. We can introduce *INNER ITERATIONS* to enforce it.

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NLRK

1: Choose a starting vector v_1 with $\|v_1\| = 1$, a starting shift λ_1 and a pole σ and set $j = 1$.
2: OUTER ITERATION
3: Set $h_j = 0; s = e_j = (0, \ldots, 0, 1)^H \in \mathbb{R}^j; x = v_j;$
4: Compute $r = A(\sigma)^{-1}A(\lambda)x$ and $k_j = V_j^H r$
5: **while** $\|k_J\| > ResTol$ **do**
6: INNER ITERATION
7: Orthogonalize $r = r - Vk_j$
8: Set $h_j = h_j + s_j^{-1}k_j$
9: Compute the smallest eigenpair (θ, s) of $H_{j,j}$
10: $x = V_j s$
11: Update $\lambda = \lambda + \frac{\theta}{1-\theta}(\lambda - \theta)$
12: Update $H_{j,j} = \frac{1}{1-\theta}H_{j,j} - \frac{\theta}{1-\theta}I$
13: Compute $r = A(\sigma)^{-1}A(\lambda)x$ and $k_j = V_j^H r$
14: **end while**
15: Compute $h_{j+1,j} = \|r\|/s_j$
16: **if** $|h_{j+1,j}s_j| > EigTol$ **then**
17: $v_{j+1} = r/\|r\|; j = j + 1;$ GOTO 3
18: **end if**
19: Store (θ, x) as eigenpair
20: If more eigenvalues are requested, choose next θ and s, and GOTO 10

Nonlinear Rational Krylov

Practical issues

This version of the algorithm works but there are two important points to make it more efficient:

- Change of pole
- Hard purging

Theorem

In $O(m^3)$ it is possible to change pole in the generalized Arnoldi sequence, in particular

$$A(\sigma)^{-1}A(\lambda)V_m = V_{m+1}H_{m+1,m} \Longrightarrow A(\bar{\sigma})^{-1}A(\bar{\lambda})W_m = W_{m+1}\widetilde{H}_{m+1,m}$$

moreover $\operatorname{span}(V_{m+1}) = \operatorname{span}(W_{m+1})$. These operations are numerically stable if σ and $\bar{\sigma}$ are far enough from the eigenvalues of the original problem.

- When enough Ritz values near a pole have converged we can change the pole.
- Heuristically a good strategy to change the pole is to take a convex combination of the next shift and the old pole.

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Nonlinear Rational Krylov

Thick restart

Let $A(\sigma)^{-1}A(\lambda)V_m = V_{m+1}H_{m+1,m}$ be an Arnoldi sequence with $\theta_1, \ldots, \theta_k$ a subset of Ritz values, where at least one has not (numerically) converged yet. Then it is possible to build another generalized Arnoldi sequence $A(\sigma)^{-1}A(\lambda)W_k = W_{k+1}\tilde{H}_{k+1,k}$ such that $\theta_1, \ldots, \theta_k$ are the Ritz values.

Hard purging

When a Ritz value has numerically converged, then all converged Ritz values and the nearest to convergence Ritz values must be locked. All the others will be purged. After that the algorithm continues.

Hard purging is heuristically proposed but it seems a necessary step of the algorithm. Without this process, the algorithm has a loop for a while on the same eigenvalue and after that it encounters a breakdown.

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Numerical experimentation

GUN problem

This is a large-scale NLEP that models a radio frequency gun cavity and is of the form

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

Where $M, K, W_1, W_2 \in \mathbb{R}^{9956\times 9956}$ are real symmetric, K is positive semidefinite, and M is positive definite. The domain of interest is

$$\Omega = \{\lambda \in \mathbb{C} \text{ such that } |\lambda - \mu| \leq \gamma \quad \text{and} \quad Im(\lambda) \geq 0\}.$$

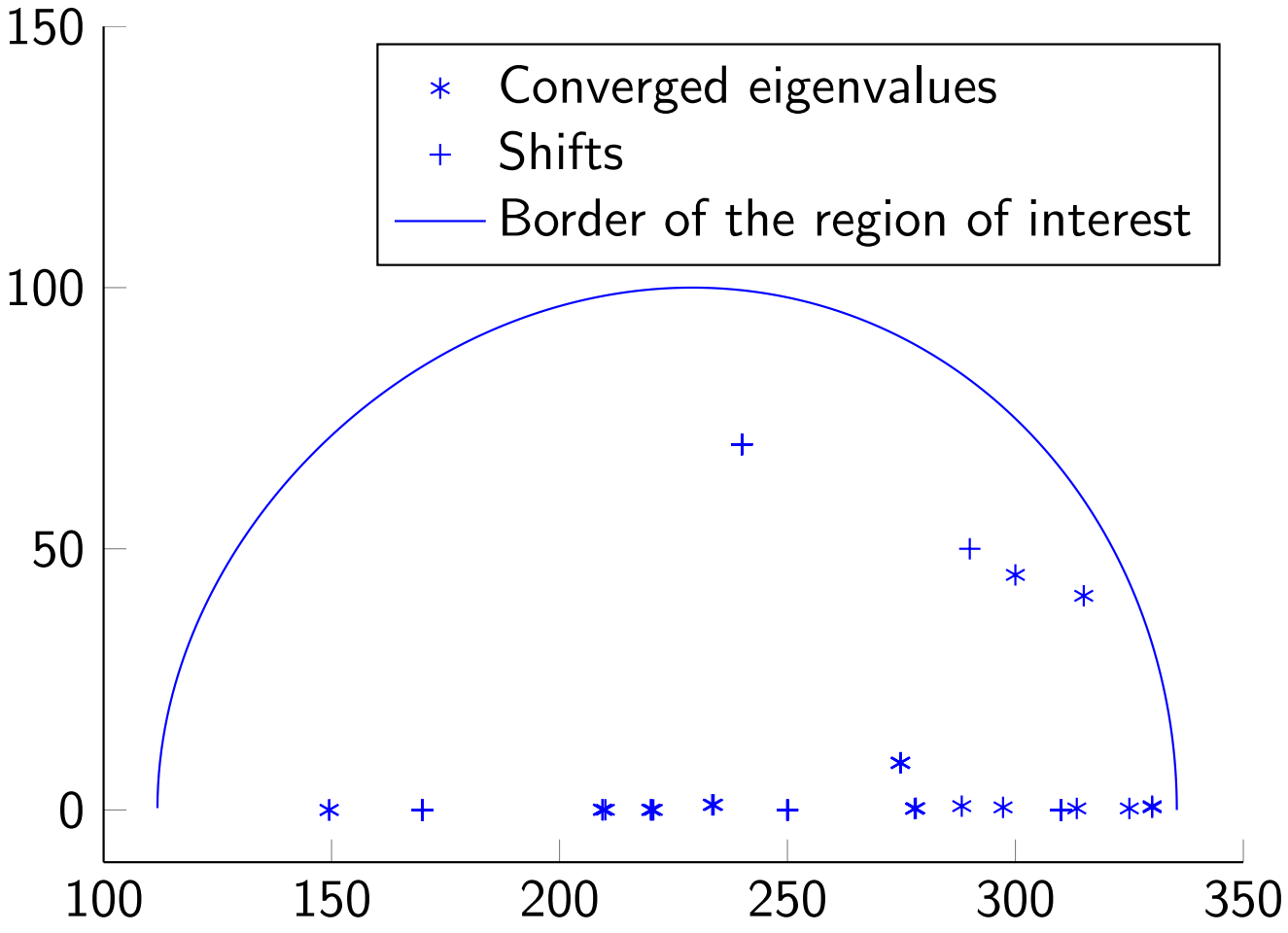
The parameters are set to $\sigma_1 = 0, \sigma_2 = 108.8774, \gamma = 50000$ and $\mu = 62500$.

Before solving the problem we applied shift and rescaling in order to transform Ω into the upper part of the unit circle.

Numerical experimentation: HIRK

- NLRK diverges
- HIRK succeeds to compute eigenvalues

Eigenvalues of the gun problem are computed with 60 iterations. The same node is used 12 times.

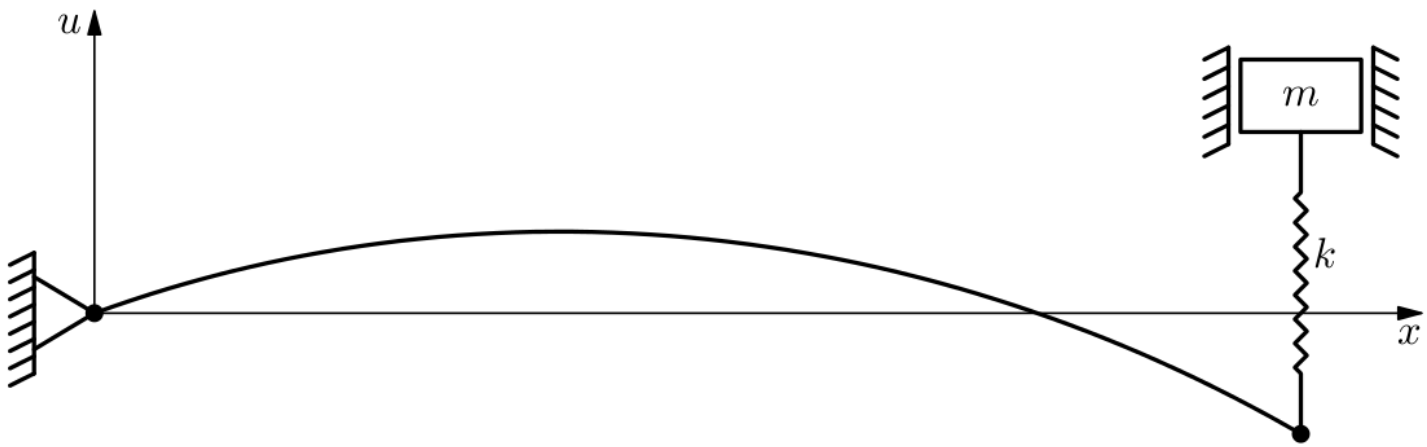


Numerical experimentation

Vibrating string with elastically attached mass

Consider the system of a limp string of unit length, which is clamped at one end. The other end is free but has a mass m attached to it via an elastic spring of stiffness k. The eigenvibrations of the string are governed by the eigenvalue problem

$$\begin{cases} -u''(x) = \lambda u(x) \\ u(0) = 0 \\ u'(1) + k\frac{\lambda}{\lambda - k/m}u(1) = 0 \end{cases}$$



Numerical experimentation

Eigenvalues of the continuum problem

With easy computations, we found that the eigenvalues are the solution of the equation

$$\tan(\sqrt{\lambda}) = \frac{1}{m\lambda} - \frac{\sqrt{\lambda}}{k}$$

Discrete problem

Discretizing the problem by means of the finite element method using $P1$ elements we arrive at the nonlinear eigenproblem

$$A - \lambda B + k\frac{\lambda}{\lambda - k/m} C = 0,$$

$$A = \frac{1}{h}\begin{pmatrix} 2 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & 2 & -1 \\ & & -1 & 1 \end{pmatrix}, \quad B = \frac{h}{6}\begin{pmatrix} 4 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & 4 & 1 \\ & & 1 & 2 \end{pmatrix}, \quad C = e_n e_n^H.$$

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Numerical experimentation: NLRK

Task

Compute the second smallest eigenvalue λ_2

Se set $EigTol = 10^{-6}$ and $ResTol = 10^{-6}$.

For $m = 1$ and $k = 0.01$ we have $\lambda_2 \simeq 2.4874$.

N	$\lvert\lambda_2 - \tilde{\lambda}_2\rvert$	Outer iterations	Average of inner iterations
100	10^{-3}	5	2
10000	10^{-5}	6	2

For $m = 1$ and $k = 0.1$ we have $\lambda_2 \simeq 2.6679$.

N	$\lvert\lambda_2 - \tilde{\lambda}_2\rvert$	Outer iterations	Average of inner iterations
100	10^{-2}	5	3
10000	10^{-3}	6	3

For $m = 1$ and $k = 1$ NLRK diverges.

HIRK succeeds to compute λ_2 but it is slow. On the other hand it works also for $m = 1$ and $k = 1$.

Numerical experimentation

Fluid-solid structure interaction

The study of free vibrations of a tube bundle immersed in a slightly compressible (under a few simplifications) leads to the following continuum eigenproblem.
Find $\lambda \in \mathbb{R}$ and $u \in H^1(\Omega_0)$ such that for every $v \in H^1(\Omega_0)$

$$c^2 \int_{\Omega_0} \nabla u \cdot \nabla v dx = \lambda \int_{\Omega_0} uv dx + \sum_{j=1^k} \frac{\lambda \rho_0}{k_j - \lambda m_j} \int_{\Gamma_j} u n ds \cdot \int_{\Gamma_j} v n ds$$

All the constants in the above problem are set equal to 1.

Discrete problem

After discretization by means of finite elements we obtain

$$A(\lambda)x = -Ax + \lambda Bx + \frac{\lambda}{1-\lambda} Cx = 0$$

where C collects the contributions of all tubes. A, B, and C are symmetric matrices, A and C are positive semidefinite, and B is positive definite

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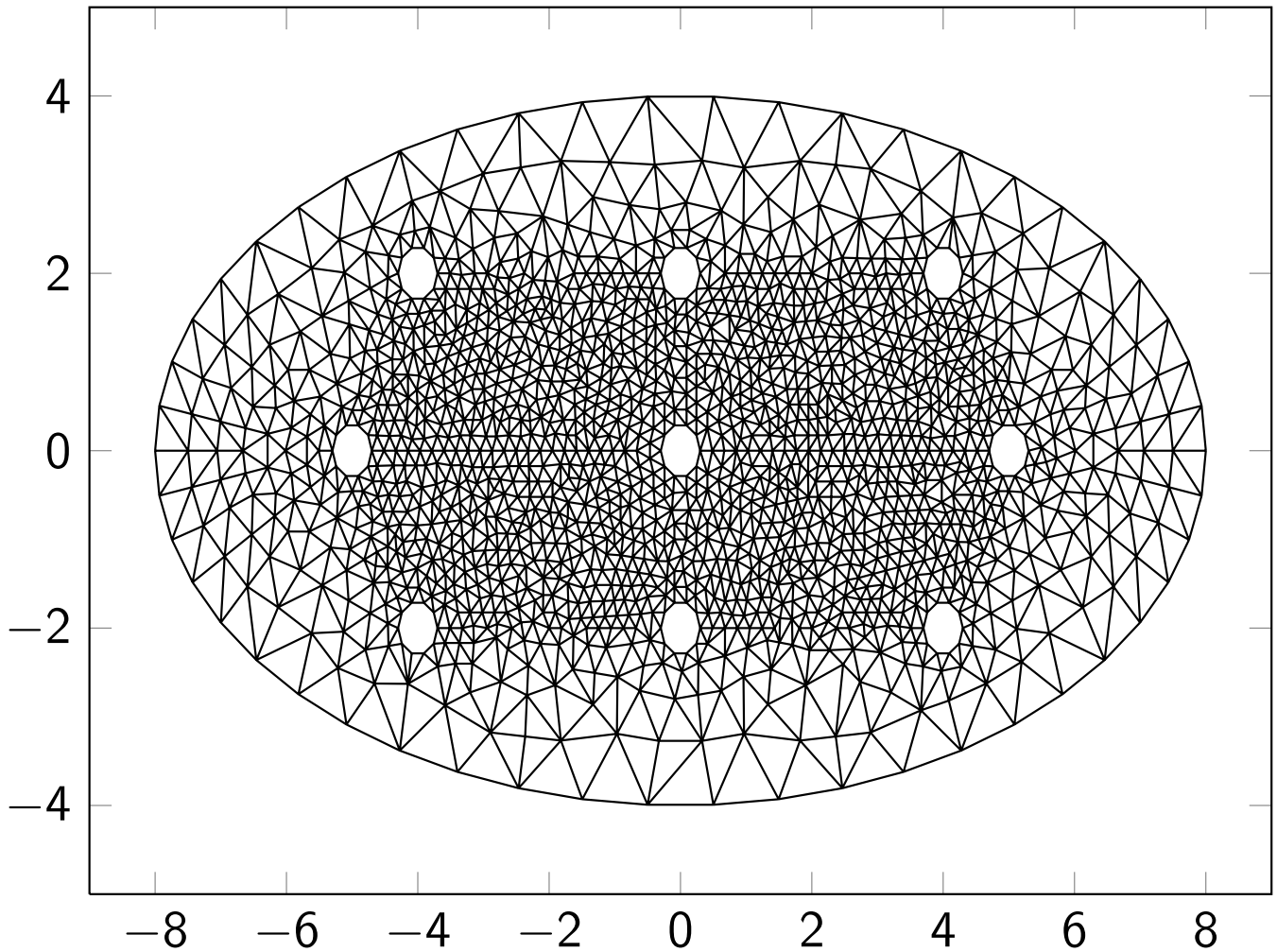
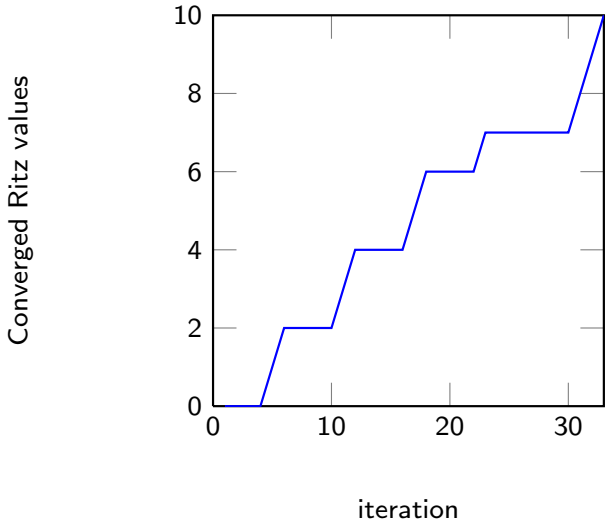
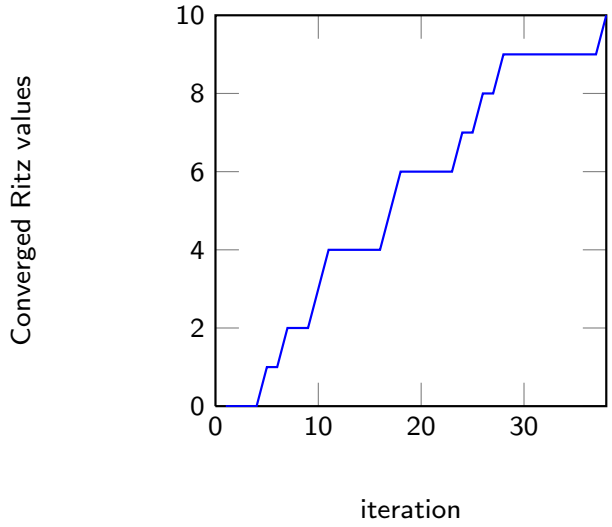
Numerical experimentation

In our setting there are 9 tubes. We discretized the problem with FreeFem++ using P1 triangular elements. Example of discretization of domain with FreeFem++

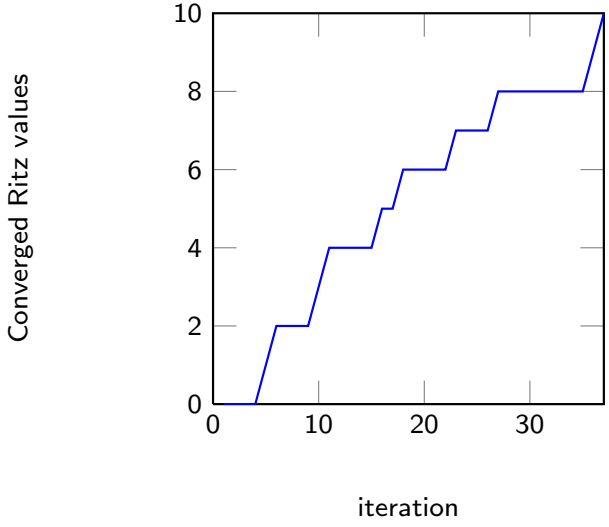




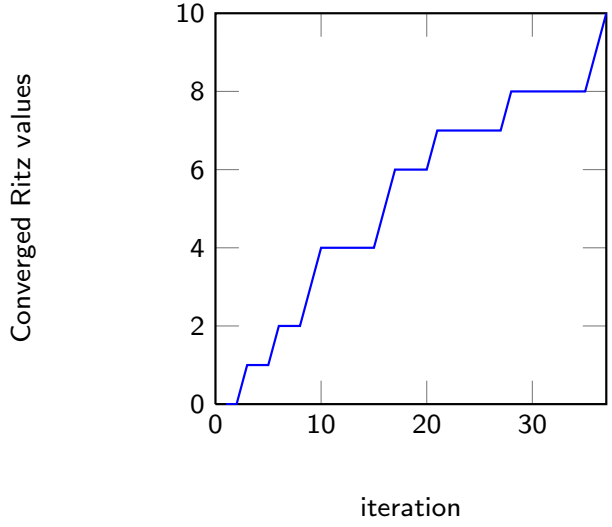
(a) $n = 50,\ m = 10,\ N = 1636$



(b) $n = 100,\ m = 10,\ N = 2156$



(c) $n = 200,\ m = 10,\ N = 3277$



(d) $n = 400,\ m = 10,\ N = 5604$

Thank you for your attention.