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ENERGY

Rational Krylov Methods for Solving Nonlinear Eigenvalue Problems

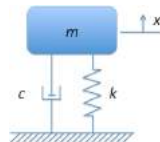
Roel Van Beeumen

`rvanbeeumen@lbl.gov`

Computational Research Division
Lawrence Berkeley National Laboratory

BASCD 2016
Stanford – December 3, 2016

Quadratic eigenvalue problem



Vibration analysis in structural analysis gives rise to

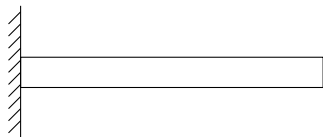
$$(\lambda^2 M + \lambda C + K)x = 0$$

where

- λ is an eigenvalue
- x is an eigenvector
- M is the mass matrix
- C is the damping matrix
- K is the stiffness matrix

Motivation: Nonlinear damping

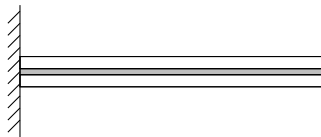
Clamped beam:



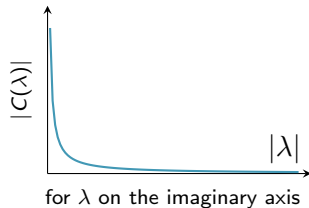
$$(\lambda^2 M + \lambda C + K) x = 0$$



Clamped sandwich beam:

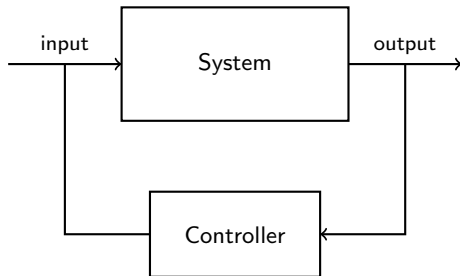


$$(\lambda^2 M + \lambda C(\lambda) + K) x = 0$$



Motivation: Active damping

Active damping in cars:



Delay eigenvalue problem

$$\left(\lambda^2 M + \lambda C + K + e^{-\lambda\tau} E \right) x = 0$$

Motivation: Nonlinear boundary conditions

Cavity design of a linear accelerator

$$\nabla \times \left(\frac{1}{\mu} \nabla \times E \right) - \lambda \epsilon E = 0$$

Maxwell's equations + nonlinear waveguide boundary conditions:

$$\left(K - \lambda M + \sum_{j=1}^k i \sqrt{\lambda - \kappa_{c,j}^2} W_j \right) x = 0$$

where

- $\lambda = \omega^2/c^2$
- $\kappa_{c,j}$ are the cutoff values

1 Motivation

2 Solving Nonlinear Eigenvalue Problems

- Approximation
- Linearization pencils
- Solving linear eigenvalue problem

3 Numerical Experiment

Nonlinear eigenvalue problem (NLEP)

NLEP

The nonlinear eigenvalue problem:

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

where

- $\lambda \in \Omega \subseteq \mathbb{C}$: eigenvalue
- $x \in \mathbb{C}^n \setminus \{0\}$: eigenvector
- $A : \Omega \rightarrow \mathbb{C}^{n \times n}$: matrix-valued function

Nonlinear eigenvalue problem (NLEP)

NLEP

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- $x \in \mathbb{C}^n \setminus \{0\}$: eigenvector
- $A : \Omega \rightarrow \mathbb{C}^{n \times n}$: matrix-valued function

Note that the NLEP is

- ↪ **nonlinear** in eigenvalue λ ,
- ↪ **linear** in eigenvector x .

Solving NLEPs

NLEP

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



PEP

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



GEP

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



Solution

① approximation via interpolation

② linearization

③ solving linear eigenvalue problem

NLEP

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



PEP

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



GEP

$$\mathbf{L}(\lambda)\mathbf{x} = 0$$



Solution

Step 1: Polynomial interpolation

$$A(\lambda) \approx P_d(\lambda) = A_0 + A_1\lambda + A_2\lambda^2 + \dots + A_d\lambda^d$$

Approximation

NLEP

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



PEP

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



GEP

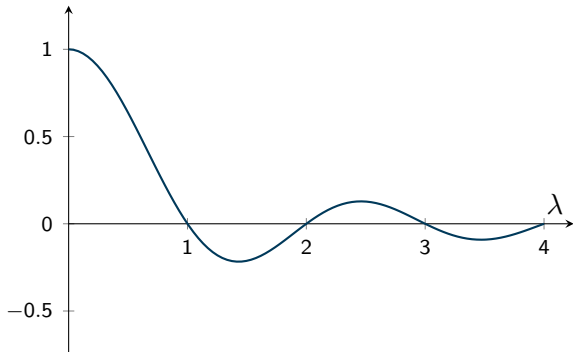
$$L(\lambda)x = 0$$



Solution

Step 1: Polynomial interpolation

$$A(\lambda) \approx P_d(\lambda) = A_0 + A_1\lambda + A_2\lambda^2 + \dots + A_d\lambda^d$$



Approximation

NLEP

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



PEP

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



GEP

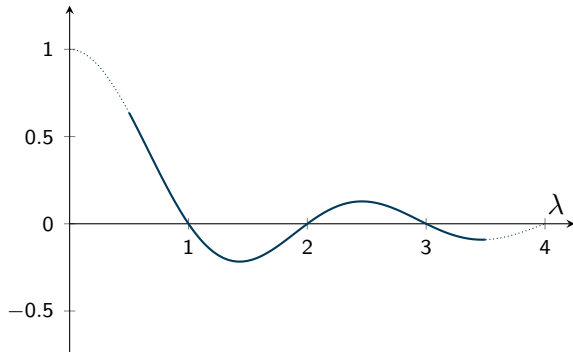
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Solution

Step 1: Polynomial interpolation

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Approximation

NLEP

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GEP

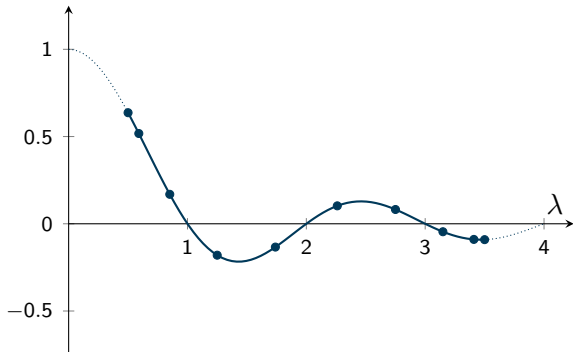
$$L(\lambda)x = 0$$



Solution

Step 1: Polynomial interpolation

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Approximation

NLEP

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



PEP

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GEP

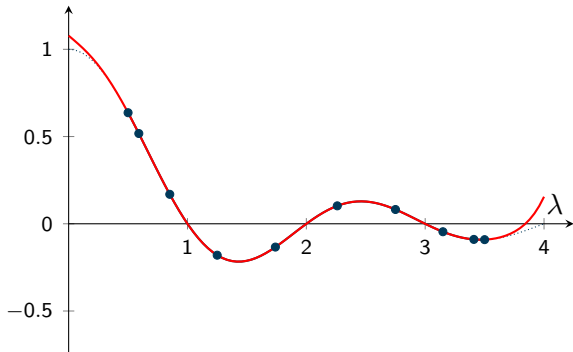
$$L(\lambda)x = 0$$



Solution

Step 1: Polynomial interpolation

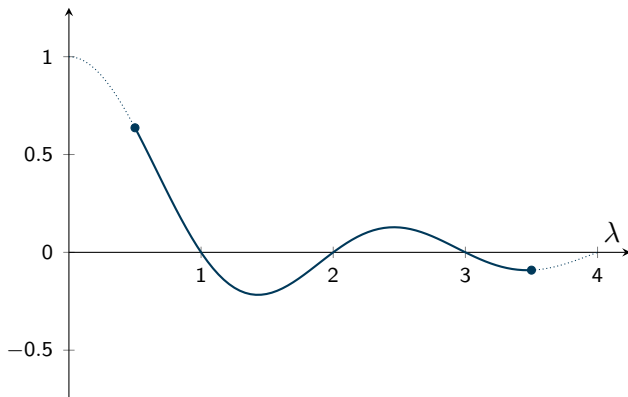
$$A(\lambda) \approx P_d(\lambda) = A_0 + A_1\lambda + A_2\lambda^2 + \dots + A_d\lambda^d$$



Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

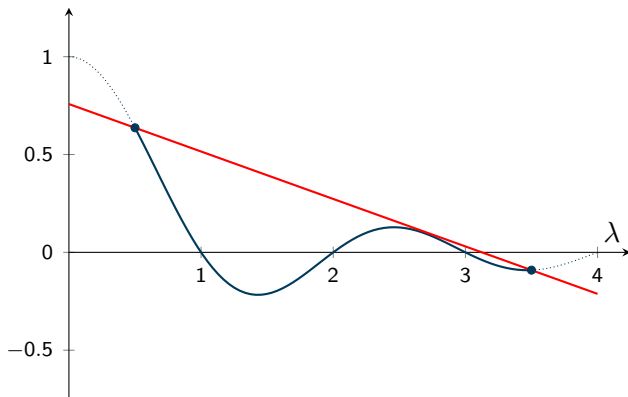
$$A(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda)$$



Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

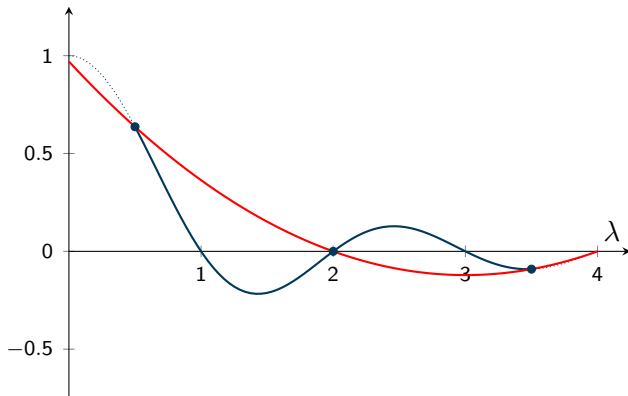
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Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

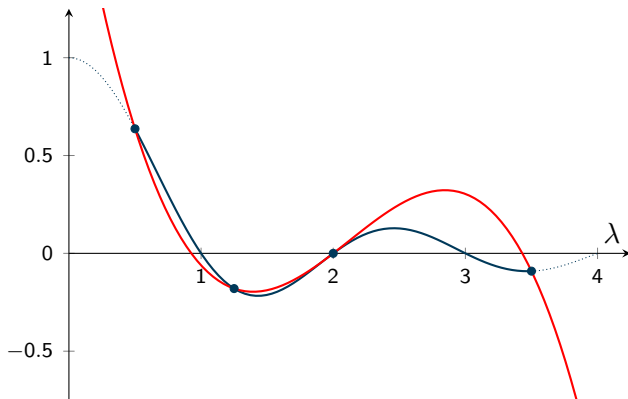
$$A(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda) + A_2 n_2(\lambda)$$



Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

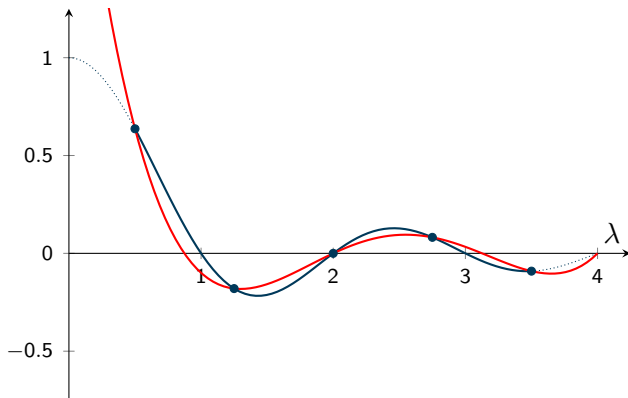
$$A(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda) + \cdots + A_3 n_3(\lambda)$$



Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

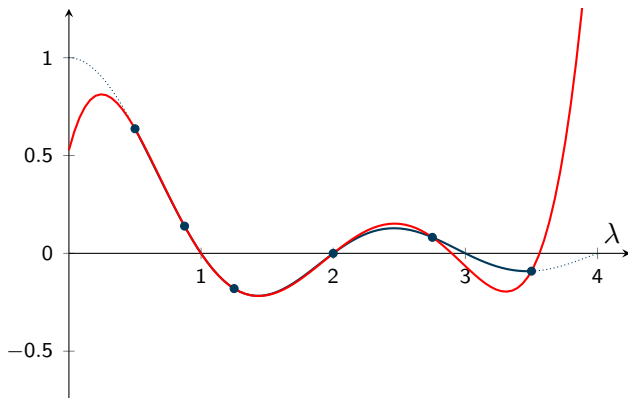
$$A(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda) + \dots + A_4 n_4(\lambda)$$



Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

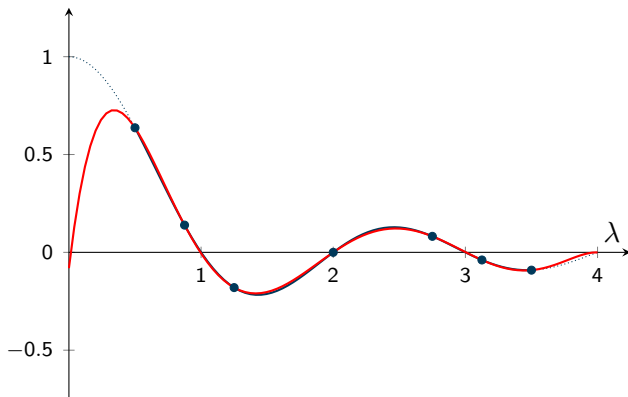
$$A(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda) + \cdots + A_5 n_5(\lambda)$$



Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

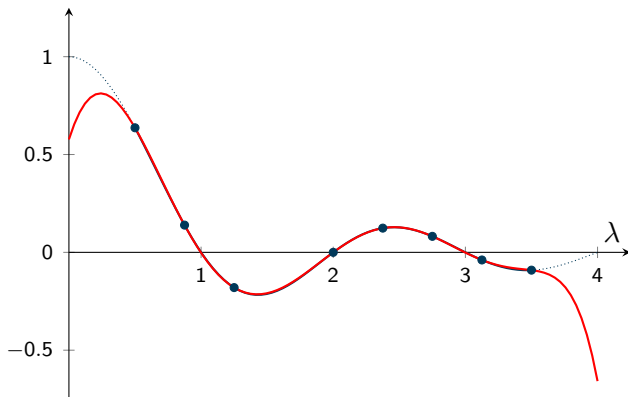
$$A(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda) + \cdots + A_6 n_6(\lambda)$$



Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

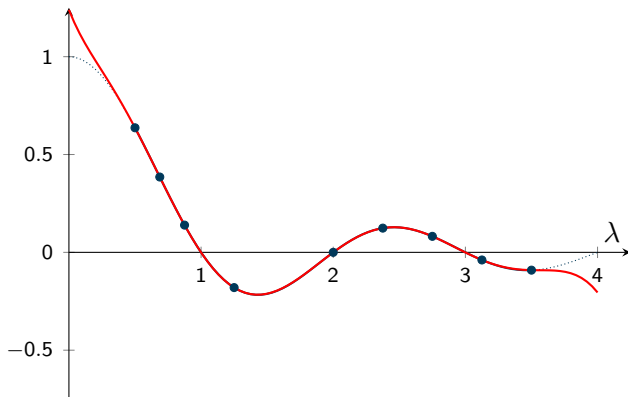
$$A(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda) + \dots + A_7 n_7(\lambda)$$



Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

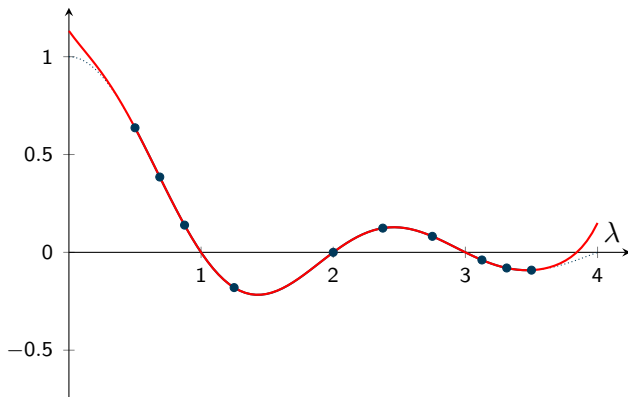
$$A(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda) + \cdots + A_8 n_8(\lambda)$$



Approximation: Newton interpolation

Dynamic polynomial interpolation (Newton)

$$A(\lambda) \approx A_0 n_0(\lambda) + A_1 n_1(\lambda) + \cdots + A_9 n_9(\lambda)$$

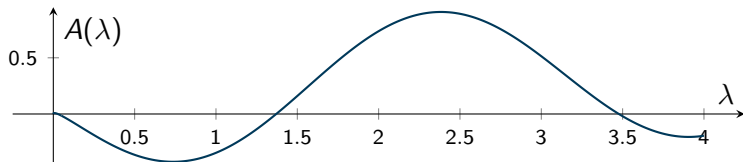


Approximation: Polynomial versus Rational

Scalar nonlinear function:

$$A(\lambda) = 0.2\sqrt{\lambda} - 0.6\sin(2\lambda) = 0$$

with target set: $\Sigma = [0.01, 4]$

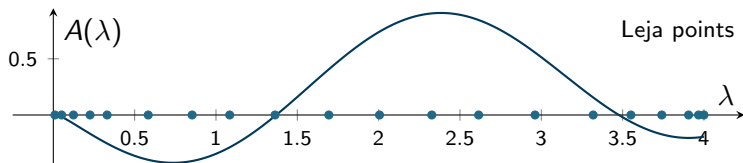


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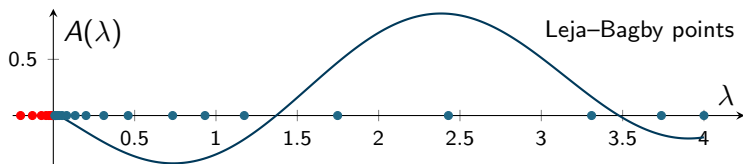
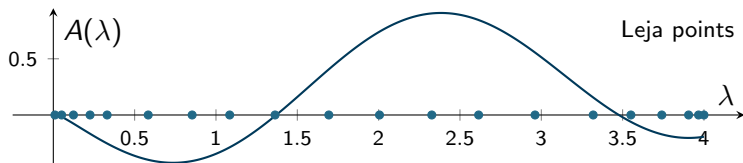


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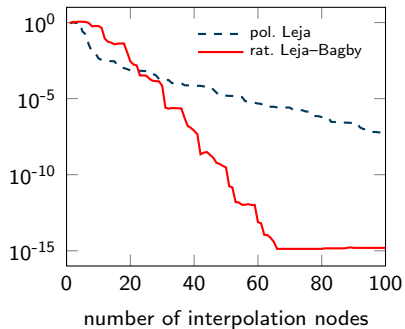


Approximation: Polynomial versus Rational

Scalar nonlinear function:

$$A(\lambda) = 0.2\sqrt{\lambda} - 0.6 \sin(2\lambda) = 0$$

interpolation error

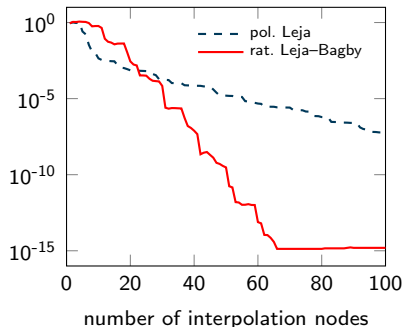


Approximation: Polynomial versus Rational

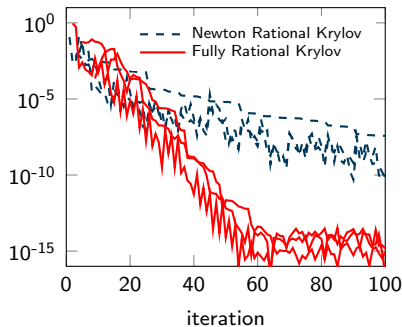
Scalar nonlinear function:

$$A(\lambda) = 0.2\sqrt{\lambda} - 0.6 \sin(2\lambda) = 0$$

interpolation error



convergence of eigenvalues



Linearization pencils

NLEP

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



PEP

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



GEP

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



Solution

Step 2: Linearization

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



$$L(\lambda)x = (\mathbf{A} - \lambda\mathbf{B})x = 0$$

Linearization: idea

Second order ODE

$$M\ddot{q} + C\dot{q} + Kq = 0$$

System of first order ODEs

$$\begin{cases} \dot{q}_1 = q_2 \\ M\dot{q}_2 = -Cq_2 - Kq_1 \end{cases}$$

$$\begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} \dot{q}_1 \\ \dot{q}_2 \end{bmatrix} = \begin{bmatrix} 0 & I \\ -K & -C \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix}$$

Linearization: idea

Second order ODE

$$M\ddot{q} + C\dot{q} + Kq = 0$$

Quadratic eigenvalue problem

$$(M\lambda^2 + C\lambda + K)x = 0$$

System of first order ODEs

$$\begin{cases} \dot{q}_1 = q_2 \\ M\dot{q}_2 = -Cq_2 - Kq_1 \end{cases}$$

$$\begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} \dot{q}_1 \\ \dot{q}_2 \end{bmatrix} = \begin{bmatrix} 0 & I \\ -K & -C \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix}$$

Linear eigenvalue problem

$$\lambda \begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 & I \\ -K & -C \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Linearization pencils

Step 2: Companion linearization

PEP

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

\Rightarrow

GEP

$$\mathbf{L}(\lambda)\mathbf{x} = (\mathbf{A} - \lambda\mathbf{B})\mathbf{x} = 0$$

$$P_d(\lambda)x = (A_0 + A_1\lambda + A_2\lambda^2 + \dots + A_d\lambda^d)x = 0$$

$$\underbrace{\begin{bmatrix} A_0 & A_1 & A_2 & \dots & A_{d-1} \\ & I & & & \\ & & I & & \\ & & & \ddots & \\ & & & & I \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_d \end{bmatrix}}_{\mathbf{x}} = \lambda \underbrace{\begin{bmatrix} 0 & 0 & \dots & 0 & -A_d \\ I & 0 & & & \\ & \ddots & \ddots & & \\ & & I & 0 & \\ & & & I & 0 \end{bmatrix}}_{\mathbf{B}} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_d \end{bmatrix}}_{\mathbf{x}}$$

Linearization pencils: Uniform representation

$$\mathbf{L}(\lambda) = \underbrace{\left[\begin{array}{cccc} A_0 & A_1 & \cdots & A_{d-1} \\ \hline & M \otimes I_n & & \end{array} \right]}_{\mathbf{A}} - \lambda \underbrace{\left[\begin{array}{cccc} B_0 & B_1 & \cdots & B_{d-1} \\ \hline & N \otimes I_n & & \end{array} \right]}_{\mathbf{B}}$$

- Monomial basis [Mackey, Mackey, Mehl, Mehrmann 2006]
- Chebyshev basis [Effenberger, Kressner 2012]
- Lagrange basis [VB, Michiels, Meerbergen 2015]
- Newton/Hermite basis [Amiraslani, Corless, Lancaster 2009]
- Rational monomial basis [Nakatsukasa, Tisseur 2014]
- Rational Newton basis [Güttel, VB, Meerbergen, Michiels 2014]
- Spectral discretization [Jarlebring, Meerbergen, Michiels 2010]
- ...

Solving linear eigenvalue problem

NLEP

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



PEP

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



GEP

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



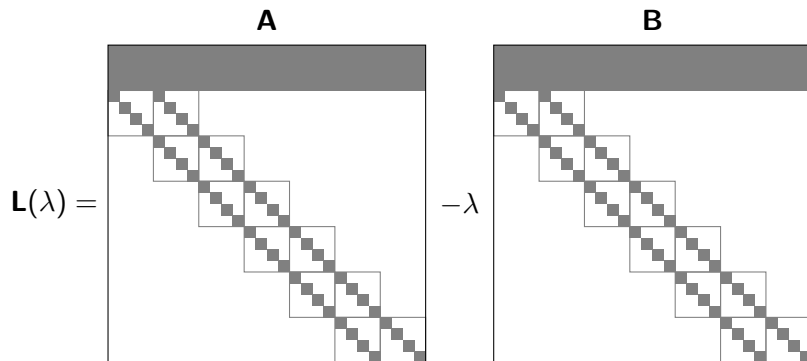
Solution

Step 3: Solve generalized linear eigenvalue problem

$$L(\lambda)x = (A - \lambda B)x = 0$$

by the rational Krylov method.

Compact Rational Krylov (CORK) framework



- full exploitation of structure \rightsquigarrow compact Krylov subspace
- reduction in memory cost
- reduction in computation cost

CORK

Generic class of numerical methods with a lot flexibility:

- polynomial or rational approximation in different bases
- interpolation nodes (and poles)
- shifts in the rational Krylov method
- dynamic / static / hybrid

Compact Rational Krylov variants:

- 1 Newton Rational Krylov (NRK) method [VB, Meerbergen, Michiels 2013]
- 2 Fully Rational Krylov (FRK) method [Güttel, VB, Meerbergen, Michiels 2014]
- 3 Infinite Arnoldi (InfA) method [Jarlebring, Michiels, Meerbergen 2012]
- 4 ...

Maxwell's equations + nonlinear waveguide boundary conditions:

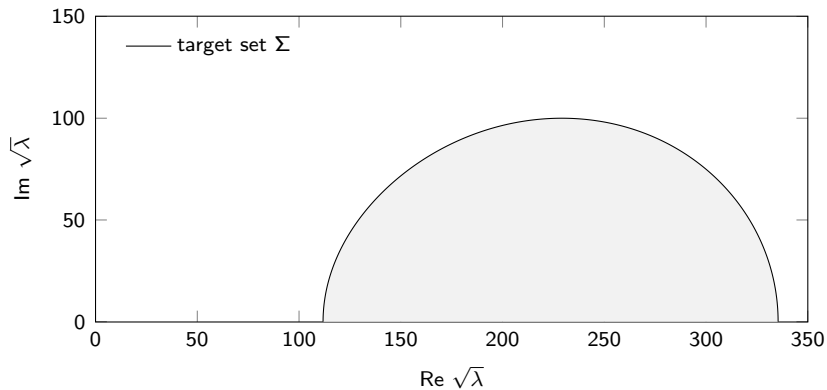
$$A(\lambda)x = \left(K - \lambda M + i\sqrt{\lambda - \alpha_1^2} W_1 + i\sqrt{\lambda - \alpha_2^2} W_2 \right) x = 0,$$

where

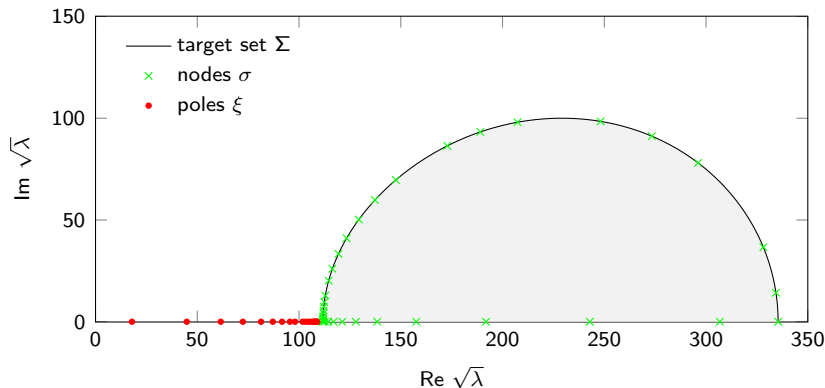
- $K, M, W_1, W_2 \in \mathbb{R}^{9956 \times 9956}$
- $\lambda = \omega^2/c^2$
 - ω the wavenumber
 - c the speed of light
- α_1 and α_2 are the cutoff values

= 'Gun' problem from the NLEVP collection

Gun problem

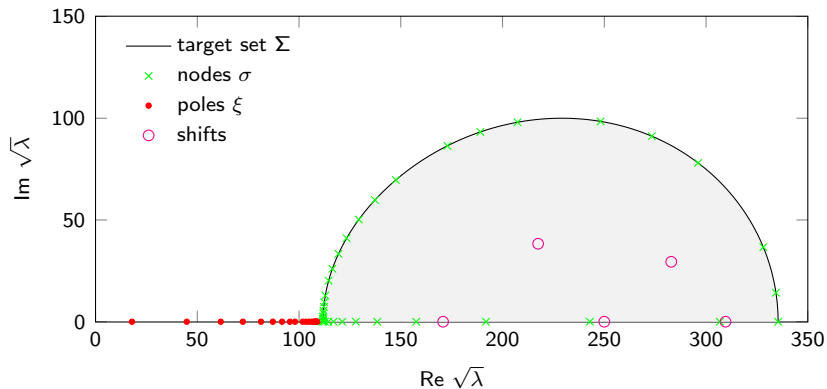


Gun problem



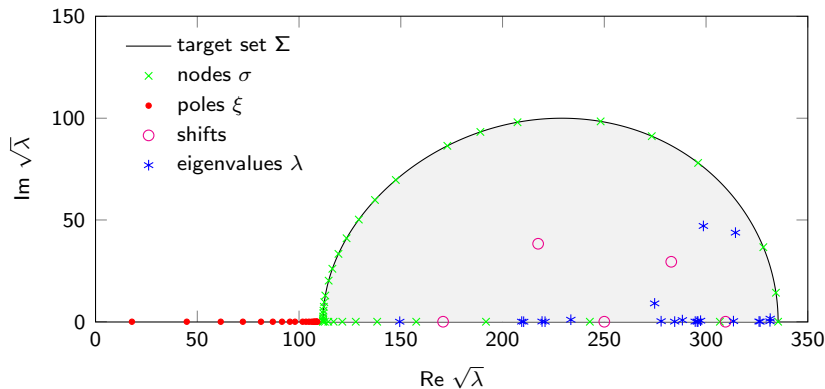
$A(\lambda)$ approximated by a rational Newton polynomial of degree $d = 35$

Gun problem



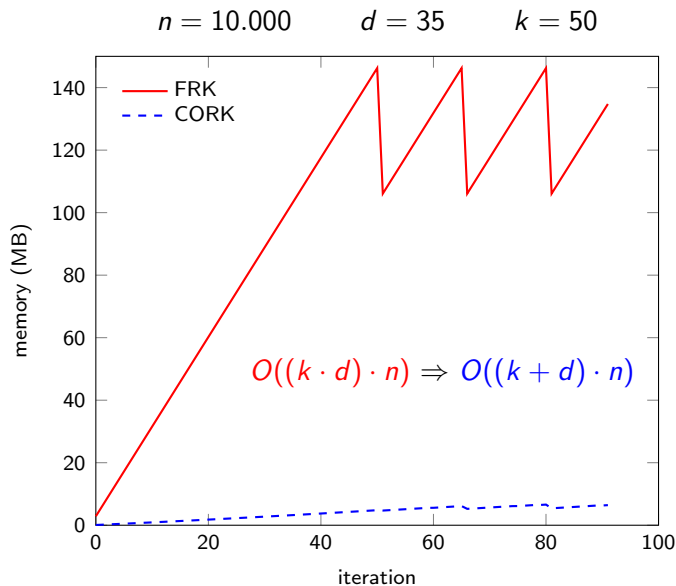
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Gun problem



$A(\lambda)$ approximated by a rational Newton polynomial of degree $d = 35$

Compact Rational Krylov (CORK) framework

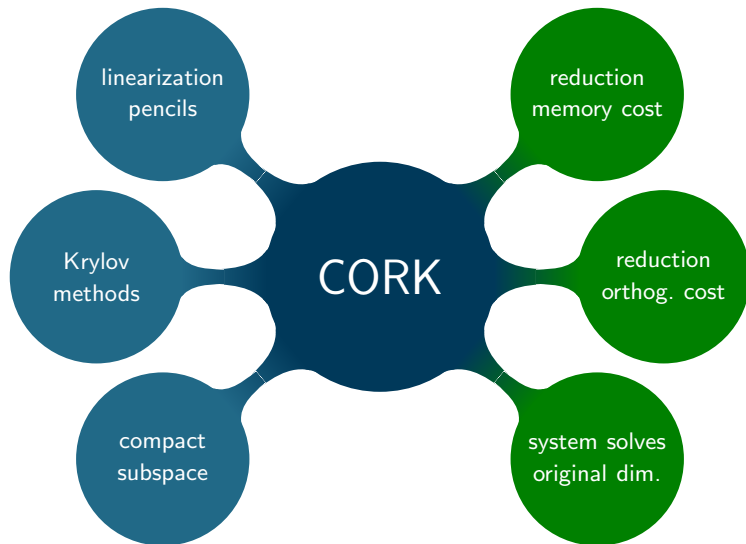


How to solve NLEP's

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

- 1 Approximation via interpolation
- 2 Linearization
- 3 Solve linear eigenvalue problem

Compact Rational Krylov (CORK) framework



- [1] VB, MEERBERGEN, AND MICHIELS. *Compact rational Krylov methods for nonlinear eigenvalue problems*
SIAM Journal on Matrix Analysis and Applications, 36(2), 820–838, 2015
- [2] GÜTTEL, VB, MEERBERGEN, AND MICHIELS. *NLEIGS: A class of fully rational Krylov methods for nonlinear eigenvalue problems*
SIAM Journal on Scientific Computing, 36 (6), A2842–A2864, 2014
- [3] VB, MEERBERGEN, AND MICHIELS. *A rational Krylov method based on Hermite interpolation for nonlinear eigenvalue problems*
SIAM Journal on Scientific Computing, 35 (1), A327–A350, 2013

CORK & NLEIGS Matlab toolboxes available on my homepage:
<http://www.roelvanbeeumen.be>

- [1] VB, MEERBERGEN, AND MICHIELS. *Compact rational Krylov methods for nonlinear eigenvalue problems*
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Thank you for your attention !