Krylov methods for eigenvalue problems: applications

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Two lectures

1. Krylov methods for eigenvalue problems: theory and algorithms
   - Concepts of spectral approximation
   - Convergence/approximation theory
   - Algorithms
2. Krylov methods for eigenvalue problems: applications
   - Nonlinear eigenvalue problems
   - Computing eigenvalues with largest real part (stability analysis of dynamical systems)

Outline of lecture 2

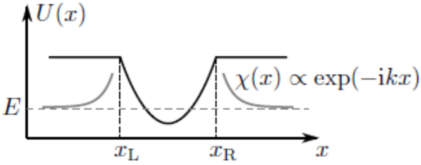
1. Nonlinear eigenvalue problem
   - Examples of nonlinear eigenvalue problems
   - Rational approximation
   - Nonlinear eigenvalue problem
   - Linearization

2. Computation of right-most eigenvalues
   - Stability analysis
   - Lyapunov Inverse Iteration
   - Related problems

Schrödinger equation

- Single particle equation

$$\left(-\frac{d^2u}{dx^2} + U(x)\right)\xi(x) = \lambda\xi(x)$$



on infinite domain

- Compute bound state (discrete part of the spectrum)
- Discrete problem:

$$(-D + \mathrm{diag}(U) + \Sigma(\lambda))X = \lambda X$$

with

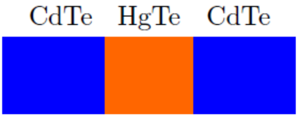
$$\begin{aligned} \Sigma &= \mathrm{diag}(\Sigma_L(\lambda), 0, \ldots, 0, \Sigma_R(\lambda)) \\ \Sigma_{L,R} &= -\frac{1}{\Delta x^2}\exp\left(i\Delta x\sqrt{\lambda - u_{L,R}}\right) \end{aligned}$$

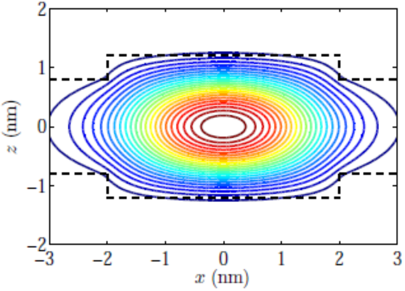
Schrödinger equation

- 2D equation

$$\left(-D + \mathrm{diag}(U) - \sum_{j=1}^{n_z} e^{0.2i\sqrt{\lambda-\alpha_j}} L_j U_j^T - \lambda I\right) x = 0$$

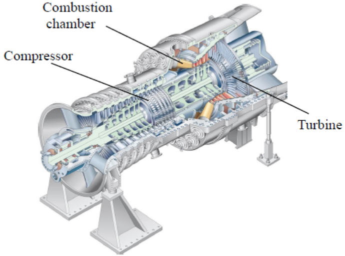
E_2 is rank $\sqrt{n}$ matrix, D is diagonal.





- Problem of dimension $n = 16,281$.
- Nonlinear part has rank $r = 162$

NEP: thermo-acoustics



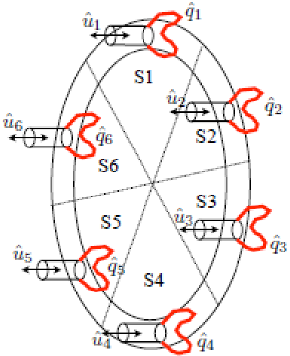
- Important industrial problem:
- Understanding (acoustic) instabilities in gas combustion turbines

Helmholtz equation for a reactive flow:

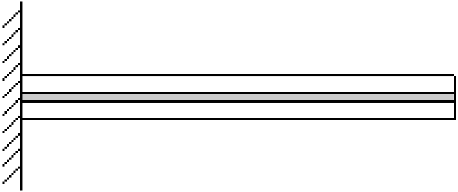
$$\nabla \cdot c_0^2 \nabla p + \omega^2 p = \eta(x,\omega) e^{i\omega\tau} \nabla p \cdot n$$

After discretization:

$$Kp - \omega^2 Mp = C(\omega)p$$



Nonlinear damping



- Clamped sandwhich beam
- 168 degrees of freedom (finite elements)
- Nonlinear eigenvalue problem:

$$\left(K_e + \frac{G_0 + G_\infty (i\omega\tau)^\alpha}{1 + (i\omega\tau)^\alpha} K_v - \omega^2 M \right) x = 0$$

with $\alpha = 0.675$ and $\tau = 8.230$.
Parameters obtained from measurements.

Nonlinear eigenvalue problem

$$A(\lambda)x = 0 \quad , \quad \lambda \in \mathbb{C}, x \in \mathbb{C}^n, x \neq 0$$

Solution methods for finding eigenvalues in a region $\Sigma \subset \mathbb{C}$:

- Residual inverse iteration and Newton's method
  [Neumaier 1998], [Kressner 2009, [Effenberger 2013], ...
  = Local approximation
- Contour integration method — 'Rational filtering'
  [Kravanja & Van Barel, 2000, 2016] [Sakurai & co.], [Polizzi & co], ...
  [Austin & Trefethen, 2015], ...
- ☛ Local and global rational approximation and linearization

Nonlinear eigenvalue problem

$$A(\lambda)x = 0 \quad , \quad \lambda \in \mathbb{C}, x \in \mathbb{C}^n, x \neq 0$$

Solution methods for finding eigenvalues in a region $\Sigma \subset \mathbb{C}$:

- ☛ Local and global rational approximation and linearization
  Assume problems of this form:

$$A(\lambda) = \sum_{j=1}^{m} A_j f_j(\lambda)$$

1. Rational Approximation

$$f_j(\lambda) \approx \frac{\alpha_0 + \ldots \alpha^p \lambda^p}{\beta_0 + \ldots \beta^p \lambda^p}$$

2. Linearization
3. Apply (rational) Krylov to the linearization

Idea of linearization

Protoytype: polynomial in monomial basis:

$$\alpha_0 + \alpha_1\lambda + \alpha_2\lambda^2 + \cdots + \alpha_d\lambda^d = 0$$

Linearization:

$$\begin{bmatrix} \alpha_0 + \alpha_1\lambda & \alpha_2\lambda & \cdots & \alpha_d\lambda^d \\ -\lambda & 1 & & \\ & \ddots & \ddots & \\ & & -\lambda & 1 \end{bmatrix} \begin{pmatrix} 1 \\ \lambda \\ \vdots \\ \lambda^{d-1} \end{pmatrix} = 0$$

(Companion linearization: linear in λ)
Other basis:
[Amiraslani, Corless & Lancaster, 2008]

Approximation 1: spectral discretization/infinite Arnoldi

Delay equation:

$$\frac{dx}{dt} = \beta_0 x + \beta_1 x(t - \tau)$$

with τ the delay
Characteristic equation:

$$\beta_0 + e^{-\lambda\tau}\beta_1 - \lambda = 0$$

Rational approximation of

$$\beta_0 + e^{-\lambda\tau}\beta_1$$

Spectral discretization Hermite interpolates at $\lambda = 0$.

Approximation 1: spectral discretization

[Michiels, Niculescu 2007], [Breda, Maset, Vermiglio 2005]

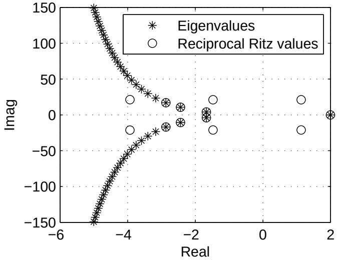
- The delay equation can be written as a linear infinite dimensional operator in $x(\theta)$ with $\theta \in [-\tau, 0]$.
- Discretization of the interval $[-\tau, 0]$
- Represent the solution on $[-\tau, 0]$ by polynomial interpolation
- With a proper basis this leads to a linearization of the form:

$$\begin{bmatrix} \rho_0 & \rho_1 & \rho_2 & \cdots & \rho_N \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix} x - \lambda \begin{bmatrix} \frac{4}{\tau} & \frac{4}{\tau} & \frac{4}{\tau} & \cdots & \frac{4}{\tau} \\ 2 & 0 & -1 & & \\ & \frac{1}{2} & 0 & \ddots & \\ & & \ddots & \ddots & -\frac{1}{N-1} \\ & & & \frac{1}{N} & 0 \end{bmatrix} x = 0$$

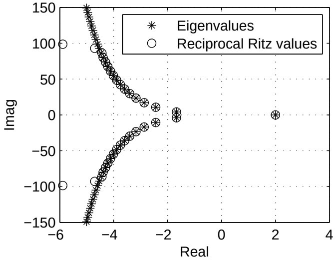
Convergence: $O(N^{-N})$

Scalar delay equation

- Comparison Taylor/infinite Arnoldi



Taylor



infinite Arnoldi

[Jarlebring, M. & Michiels, 2010, 2012]

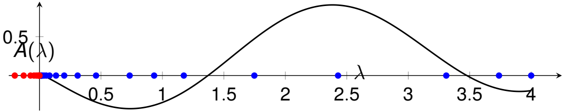
Approximation 2: potential theory

- Build a rational approximation, expressed in rational Newton polynomial basis
- Choice of interpolation points and poles
- Potential theory: Leja (Bagby) points for finding roots in $\Sigma \in \mathbb{C}$:
  - Choose poles in the singularity set of $f(\lambda)$ (away from Σ)
  - Interpolation points are chosen so that the approximation error satisfies a *signed equilibrium measure*. (See talk by Françoise.)

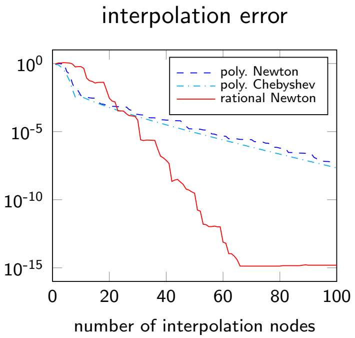
  [Bagby 1969], [Walsh, 1932, 1966, 1969].
- The poles are dependent on the function
- Interpolation points are independent of the function!
- Scaling of the rational Newton polynomials
- Code: NLEIGS

Potential theory: choosing interpolation points

Nonlinear function: $f(\lambda) = 0.2\sqrt{\lambda} - 0.6\sin(2\lambda) = 0$ on $\Sigma = [0.01, 4]$



- interpolation points are Leja Bagby points in $[10^{-2}, 4]$
- the poles lie in the branch cut of $\sqrt{\lambda}$ (away from the interval)



[Güttel, Van Beeumen, M., & Michiels, 2013]

Approximation 3: Representation in state space form

- Rational polynomial representation:

$$\alpha + \lambda\beta + \frac{p(\lambda)}{q(\lambda)} = \alpha + \lambda\beta - a^T(C - \lambda D)^{-1}b$$

- Linearization:

$$\begin{bmatrix} \alpha + \lambda & a^T \\ b & C - \lambda D \end{bmatrix} \begin{pmatrix} 1 \\ -(C - \lambda D)^{-1}b \end{pmatrix} = 0$$

  [Su & Bai, 2011]
- [Su & Bai, 2011] use a Padé approximation: approximation around $\lambda = 0$: suitable with shift-and-invert Arnoldi.
- Rational approximation by AAA-method [Lietaert, M., Perez, Vandereycken, 2017]

pproximation 3: Representation in state space form

Idea of AAA:

- Nakatsukasa, Sète and Trefethen 2016
- Rational approximation in barycentric form:

$$r(\lambda) = \underbrace{\sum_{j=1}^{m} \frac{f_j \omega_j}{\lambda - z_j}}_{=:n_m(\lambda)} \Big/ \underbrace{\sum_{j=1}^{m} \frac{\omega_j}{\lambda - z_j}}_{=:d_m(\lambda)},$$

  interpolates f in $z_1, \ldots, z_m$.
- Iterative procedure that select points following a greedy approach.
- Points are selected from a user defined set $Z_M \subset \Sigma$ with $M \gg 1$
  The rational function can be written in the form

$$r(\lambda) = a^T (C - \lambda D)^{-1} b$$

Nonlinear eigenvalue problem

$$A(\lambda)x = 0 \quad \text{for} \quad \lambda \in \Gamma$$

Here, we assume the following form:

$$A(\lambda) = \sum_{j=1}^{m} A_j f_j(\lambda)$$

Three steps:

1. polynomial approximation

$$A(\lambda) \approx \sum_{j=0}^{d} A_j p_j(\lambda) \quad \text{on } \Gamma$$

   with p_j (rational) polynomial of degree d.
   Use infinite Arnoldi, Padé, AAA, NLEIGS, …
2. linearization
3. solution

Linearization

Polynomial formulation:

$$A(s) = \sum_{j=0}^{d-1} (A_j - sB_j)\phi_j(s) \in \mathbb{C}^{n\times n}$$

with ϕ_j scalar functions and A_j, B_j constant matrices.

Linearization

Polynomial formulation:

$$A(s) = \sum_{j=0}^{d-1} (A_j - sB_j)\phi_j(s) \in \mathbb{C}^{n\times n}$$

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CORK Linearization:

$$\begin{aligned} \mathbf{L}(s) &= \mathbf{A} - s\mathbf{B} \\ &= \left[\begin{array}{cccc} A_0 - sB_0 & A_1 - sB_1 & \cdots & A_{d-1} - sB_{d-1} \\ \hline \multicolumn{4}{c}{(M - sN) \otimes I_n} \end{array} \right] \end{aligned}$$

with $M - sN$ linear dual basis:

$$(M - sN)\Phi = 0 \quad \Phi = \begin{pmatrix} \phi_0 \\ \vdots \\ \phi_d \end{pmatrix}$$

Compact rational Krylov decomposition

[Su, Zhang, Bai 2008], [Zhang, Su 2013] & [Kressner, Roman 2013], [Van Beeumen, M. & Michiels, 2014], [Gonzáles Pizarro & Dopico, 2017]

The iteration vectors:

$$\mathbf{V} = \begin{bmatrix} v_{11} & v_{12} & \cdots & v_{1,j+1} \\ v_{21} & v_{22} & \cdots & v_{2,j+1} \\ \vdots & \vdots & \ddots & \vdots \\ v_{d1} & v_{d2} & \cdots & v_{d,j+1} \end{bmatrix}$$

- Define Q such that

$$\text{span}(Q) = \text{span}\left\{\begin{bmatrix} v_{11} & \cdots & v_{1,j+1} & \cdots & v_{d1} & \cdots & v_{d,j+1} \end{bmatrix}\right\}$$

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  with

$$r := \operatorname{rank}(Q) \leq d + j.$$

- Storage cost: $n \cdot d \cdot j \Longrightarrow n \cdot (d + j)$

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The iteration vectors:

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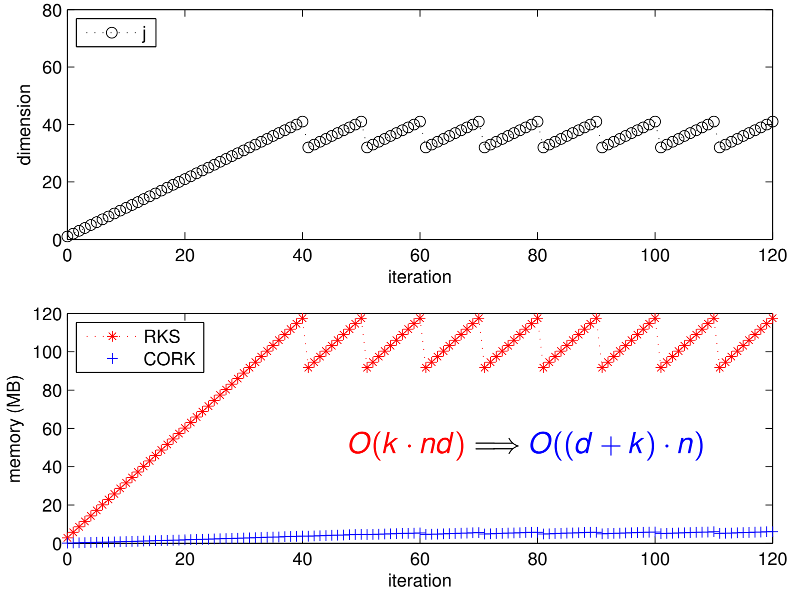
Numerical experiments

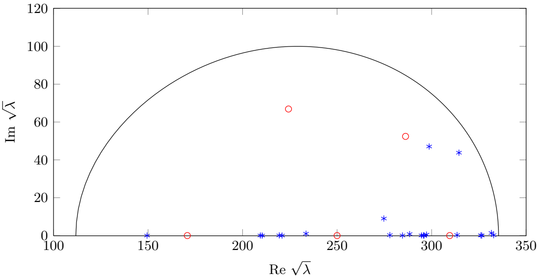


$$O(k \cdot nd) \Longrightarrow O((d + k) \cdot n)$$

Example: NLEVP's Gun problem

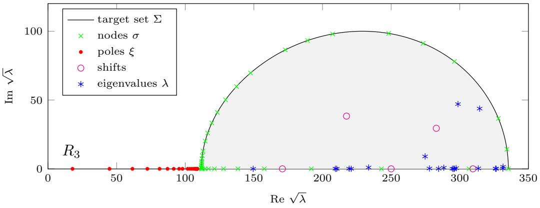
$$A(\lambda)x = \left(K - \lambda M + i\sqrt{\lambda - \alpha_1^2}W_1 + i\sqrt{\lambda - \alpha_2^2}W_2\right)x = 0,$$

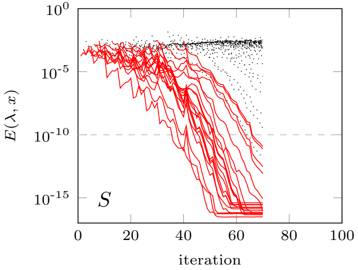
where $A(\lambda) \in \mathbb{C}^{9956 \times 9956}$.
Goal: compute all eigenvalues in a halve circle in the λ-plane.



Approximation with Leja-Bagby points (NLEIGS)

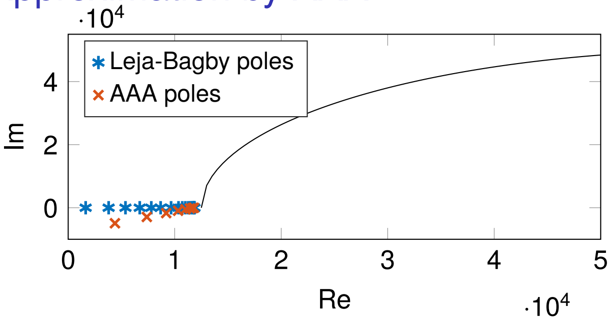
- Choose interpolation nodes σ_j and poles ξ_j for $j = 1, \ldots, N$ with N such that f_i are well approximated by rational polynomials of degree N (as for contour integral methods).

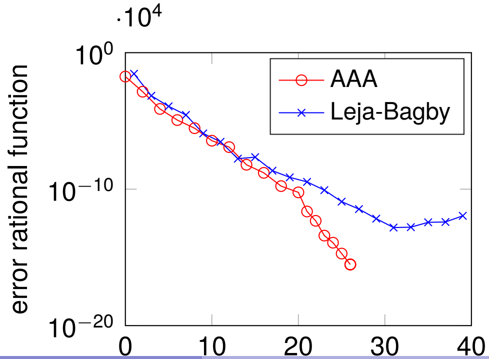




- Rational Krylov using the five poles poles in the interior.

Approximation by AAA





Summary

- General approach:
  1. Approximate $A(\lambda)$ by a (rational) polynomial
  2. Write down a linearization
  3. Use a Krylov method for solving the linearization exploiting its structure.
- Some knowledge about the nonlinear functions is required.
  - For eigenvalues in a region: use AAA, NLEIGS, or contour integration
  - For eigenvalues near a point or a line: use infinite Arnoldi or Padé approximation
- Rather involved to programme yourself
  Software in the works

Detection of Hopf bifurcations

- Nonlinear dynamical system with a parameter $\gamma \in \mathbb{R}$

$$M\frac{du}{dt} = f(u, \gamma) \quad , u(0) = u_0$$

- M: mass matrix
- f: operator in $(\mathbb{R}^n, \mathbb{R}) \mapsto \mathbb{R}$
- n is large
- Stability analysis of the steady state solution
- Find γ so that steady state corresponds to a Hopf bifurcation

Detection of Hopf bifurcations

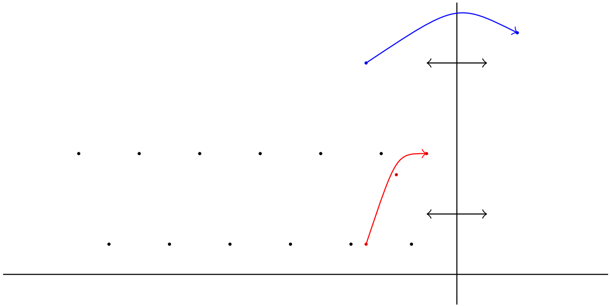
- Popular method: linearized stability analysis

$$(A + \gamma B)x = \lambda Mx$$

  where $A + \gamma B$ is the Jacobian of f evaluated at the steady state corresponding with γ
- Hopf bifurcation: two purely imaginary eigenvalues and the other eigenvalues lie in the left half plane

Detection of Hopf bifurcations

- Monitor the right-most eigenvalue as a function of γ



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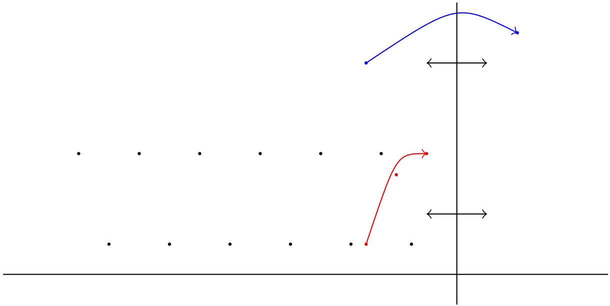

- Continuation of eigenvalues [Bindel, Demmel, Friedman 2008]

Detection of Hopf bifurcations

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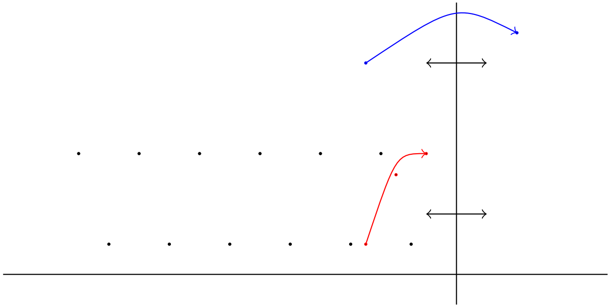

- Continuation of eigenvalues [Bindel, Demmel, Friedman 2008]
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Detection of Hopf bifurcations

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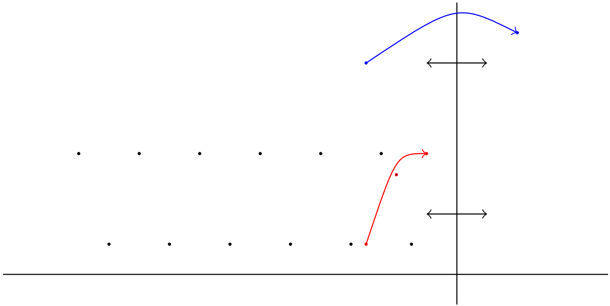

- Continuation of eigenvalues [Bindel, Demmel, Friedman 2008]
- Risk of missing eigenvalues
- Finding rightmost eigenvalues is hard: most eigenvalue solvers compute eigenvalues near a point

Detection of transition from stable to unstable branches

- Assume that for $\gamma = 0$, $(A + \gamma B)x = \lambda Mx$ has only stable eigenvalues.
  We are looking for the first γ that produces an unstable steady state.

Detection of transition from stable to unstable branches

- Assume that for $\gamma = 0$, $(A + \gamma B)x = \lambda Mx$ has only stable eigenvalues.
  We are looking for the first γ that produces an unstable steady state.

- Detection of unstable branches by transition of real eigenvalues through the origin is an easy problem to solve:
  Find γ, x so that $(A + \gamma B)x = 0$
- Not so easy for a Hopf point, since λ is an additional unknown:
  $(A + \gamma B)x = \lambda Mx$

Two-parameter eigenvalue problem

- Given x and λ so that $(A + \gamma B)x = \lambda Mx$ with λ purely imaginary.
- Then

$$(A + \gamma B)\bar{x} = -\lambda M\bar{x}$$

- and by bringing them together

$$(A + \gamma B)x - \lambda Mx = 0$$
$$(A + \gamma B)\bar{x} + \lambda M\bar{x} = 0$$

This a is two-parameter eigenvalue problem

Solving the two-parameter eigenvalue problem

- Solution of the two-parameter eigenvalue problem by Jacobi-Davidson style methods (= Newton's method) [Hochstenbach, Kosir, Plestenjak 2005]

$$\begin{aligned} A_1 z_1 &= \lambda B_1 z_1 + \mu C_1 z_1 \\ A_2 z_2 &= \lambda B_2 z_2 + \mu C_2 z_2 \end{aligned}$$

- This method starts from guesses of γ and λ
  - For γ, we can use $\gamma = 0$, since we are looking for the smallest γ.
  - A good starting guess of λ is *not* so easy to find;

Kronecker Eigenvalue Problem (KEVP)

Theorem

$$\begin{aligned}(A+\gamma B)x &= \lambda Mx \\ (A+\gamma B)\bar{x} &= -\lambda M\bar{x}\end{aligned}$$

$$\Downarrow$$

$$((A+\gamma B)\otimes M + M\otimes(A+\gamma B))\,x\otimes\bar{x} = 0$$

- Small scale problems [Guckerheimer et al. 1993, 1997] [Govaerts, 2000]
- Bialternate product:

$$\frac{1}{2}((A+\gamma B)\otimes I + I\otimes(A+\gamma B))$$

has a pair of zero eigenvalues when $A+\gamma B$ has a pair of purely imaginary eigenvalues. (case $M=I$)

Solving the Kronecker eigenvalue problem

- Kronecker problem:

$$((A+\gamma B)\otimes M + M\otimes(A+\gamma B))(x\otimes y) = 0 \qquad n^2\times n^2$$

  (No need for λ!)
- QR-method $\rightarrow O(n^6)$: only small problems
- Arnoldi $\rightarrow O(n^3)$ per iteration and n^2-vectors
  - Solve Kronecker system using Bartels-Stewart.
- For large scale problems: storage of n^2-vectors is not feasible
  - Use special variant of inverse iteration
  - Solve Kronecker system using (rational) Krylov methods.
  - Can impose structure on the eigenvector (manifold method)

Inverse iteration for KEVP

- Solution of $(A + \gamma B) \otimes Mz + M \otimes (A + \gamma B)z = 0$
- Inverse iteration:
  1. Solve y_{k+1} from $(A \otimes M + M \otimes A)y_{k+1} = (B \otimes M + M \otimes B)z_k$
  2. Normalize $z_{k+1} = y_{k+1}/\|y_{k+1}\|_2$

Inverse iteration for KEVP

- Solution of $(A+\gamma B)\otimes Mz + M\otimes(A+\gamma B)z = 0$
- Inverse iteration:
  1. Solve y_{k+1} from $(A\otimes M + M\otimes A)y_{k+1} = (B\otimes M + M\otimes B)z_k$
  2. Normalize $z_{k+1} = y_{k+1}/\|y_{k+1}\|_2$
- Represent $z_k \in \mathbb{R}^{n^2}$ by $Z_k \in \mathbb{R}^{n\times n}$ with $z_k = \mathrm{vec}(Z_k)$.
- Solve the Lyapunov equation:
  1. Solve Y_{k+1} from $AY_{k+1}M^T + MY_{k+1}A^T = BZ_kM^T + MZ_kB^T$
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Inverse iteration for KEVP

- Solution of $(A + \gamma B) \otimes Mz + M \otimes (A + \gamma B)z = 0$
- Inverse iteration:
  1. Solve y_{k+1} from $(A \otimes M + M \otimes A)y_{k+1} = (B \otimes M + M \otimes B)z_k$
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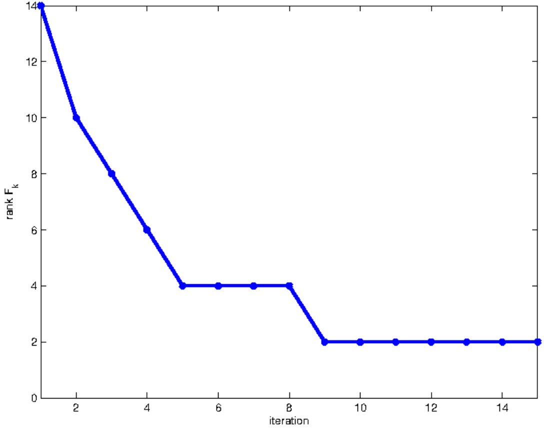
- Advantage of this approach:
  - Inverse iteration converges to an eigenvector: $x \otimes \bar{x} + \bar{x} \otimes x$
  - Which is represented by a rank two matrix: $\bar{x}x^T + x\bar{x}^T$
  - Low rank solution of Lypaunov equation can be stored.

Lyapunov solvers

- Solve Y from
$$AYM^T + MYA^T = C$$
- Small scale matrices:
  - Bartels and Stewart method, 1972
- Large scale matrices:
  - Working with full matrices is impractical for large problems
  - Approximate Lyapunov solution by a low rank matrix
  $$Y = V_k D_k V_k^T$$
  with $V \in \mathbb{R}^{n\times k}$, $k \ll n$ and $V^T V = I$.
  - Krylov methods (extended Krylov methods) [Many papers]
  - Rational Krylov type, ADI/Smith type methods [Many papers]

Rank of iterates



Inverse iteration for KEVP

Difficulties:

- Lyapunov solvers assume a low rank right-hand side for efficient computation.

Inverse iteration for KEVP

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- Lyapunov solvers assume a low rank right-hand side for efficient computation.
- Force the iterate to have rank two at every iteration:
    1. Solve Y_{k+1} from $AY_{k+1}M^T + MY_{k+1}A^T = BZ_kM^T + MZ_kB^T$
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    3. Normalize $Z_{k+1} = Y_{k+1}/\|Y_{k+1}\|_F$

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  2. Force Y_{k+1} to rank two
  3. Normalize $Z_{k+1} = Y_{k+1}/\|Y_{k+1}\|_F$
- How do we force rank two?
  - Rank two truncation of Y_{k+1} is not a good idea
  - Projection trick

Projection trick

- Let eigenvector iterate be $Z = VDV^T$ with $V \in \mathbb{R}^{n \times k}$.
- Define the 'Galerkin projected' KEVP:

$$((\widehat{A} + \gamma\widehat{B}) \otimes \widehat{M} + \widehat{M} \otimes (\widehat{A} + \gamma\widehat{B}))\widehat{z} = 0$$

  with $\widehat{A} = V^TAV$, $\widehat{B} = V^TBV$, and $\widehat{M} = V^TMV$, and $\widehat{z} \in \mathbb{R}^{k^2}$
- This is a small scale problem that can be solved by the QR method or Arnoldi.
- Galerkin solution: $(V \otimes V)\widehat{z}$.
- Two advantages:
  - $(V \otimes V)\widehat{z}$ has rank at most two
  - $(V \otimes V)\widehat{z}$ is usually a better approximation than Z.

Navier-Stokes

- Navier-Stokes equation

$$\begin{aligned} u_t &= \nu\nabla^2 u - u\cdot\nabla u - \nabla p \\ 0 &= \nabla\cdot u \end{aligned}$$

- Finite element discretization (IFISS) leads to the Jacobian

$$A + \nu B$$

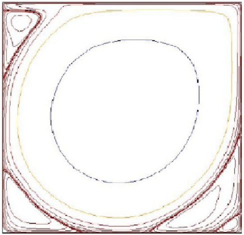
- The eigenvalue problem is

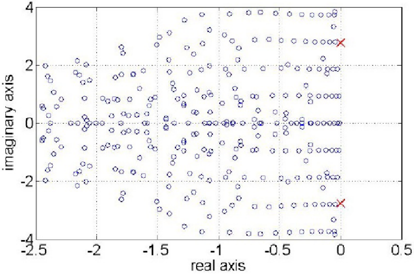
$$\begin{bmatrix} K_0+\nu K_1 & C \\ C^T & 0 \end{bmatrix}\begin{pmatrix} u \\ p \end{pmatrix} = \lambda \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}\begin{pmatrix} u \\ p \end{pmatrix}$$

  where ν is the parameter

Driven cavity

- IFISS, $Q_2 - Q_1$ mixed finite elements, $128 \times 128 \Rightarrow n = 37,507$
- Streamlines of steady solution and spectrum:





- Computation of critical Reynolds number around 8000.
- This is a difficult problem

Driven cavity

- Starting point $\text{Re}_0 = 7800$
- $\mathcal{R}$: residual KEVP, R: residual Lyapunov equation
- Lyapunov equation solved so that $\|R\|_F \leq 10^{-1}\|\mathcal{R}\|_F$
- 4 iterations:

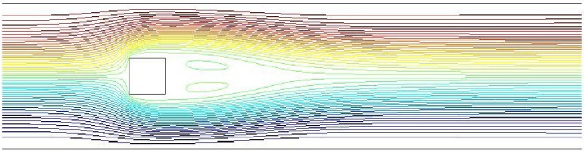
γ	λ	$\|\mathcal{R}\|$	$\|R\|_F$	m	k
-219	$2.65 \cdot 10^{-12}$	$4.94 \cdot 10^{1}$	$4.79e \cdot 10^{0}$	510	120
8173	$2.81562i$	$2.57 \cdot 10^{-2}$	$2.44 \cdot 10^{-3}$	536	190
8083	$2.80915i$	$3.58 \cdot 10^{-4}$	$3.38 \cdot 10^{-5}$	552	210
8077	$2.80960i$	$2.07 \cdot 10^{-5}$	$2.01 \cdot 10^{-6}$	532	210

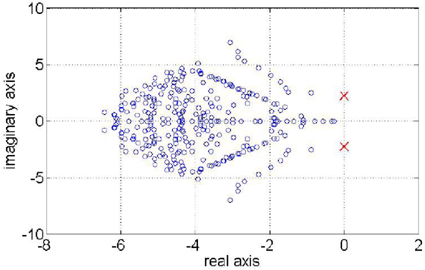
Fast convergence!

[Elman, M., Spence & Wu, 2012]

Obstacle in flow

- IFISS, $Q_2 - Q_1$ mixed finite elements, $128 \times 512 \Rightarrow n = 146,912$
- Streamlines of steady solution and spectrum:





- Computation of critical Reynolds number around 372.
- This is an easy problem

Obstacle in flow

- Starting point $\mathrm{Re}_0 = 320$
- $\mathcal{R}$: residual KEVP, R: residual Lyapunov equation
- Lyapunov equation solved so that $\|R\|_F \leq 10^{-1}\|\mathcal{R}\|_F$
- 6 iterations:

γ	λ	$\|\mathcal{R}\|$	$\|R\|_F$	m	k
-331	$-6.21 \cdot 10^{-13}$	$4.38 \cdot 10^{0}$	$4.22e \cdot 10^{-1}$	202	30
366	$2.21977i$	$3.67 \cdot 10^{-2}$	$3.34 \cdot 10^{-3}$	84	40
368	$2.26650i$	$3.77 \cdot 10^{-3}$	$2.59 \cdot 10^{-4}$	80	30
374	$2.26727i$	$5.17 \cdot 10^{-4}$	$3.17 \cdot 10^{-5}$	80	30
373	$2.26650i$	$5.51 \cdot 10^{-5}$	$5.22 \cdot 10^{-6}$	76	40
373	$2.26657i$	$5.34 \cdot 10^{-6}$	$4.04 \cdot 10^{-7}$	76	40

Fast convergence!

Related problems

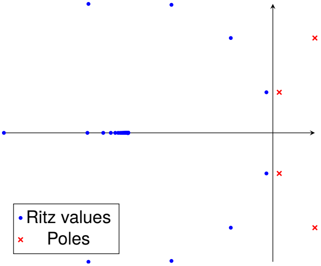
- Nearest multiple eigenvalue
- Similar ideas were used by [Gu, Mengi, Overton, Xia, Zhu, 2006] to estimate the distance to controllability
- And by [Michiels & Niculescu 2007], [Jarlebring 2008]
- [Jarlebring & Hochstenbach, 2009] formulate two-parameter eigenvalue problems for critical delays
- [M., Schröder & Voss 2013] present a structure preserving Jacobi-Davidson method for determining critical delays
- Eigenvalues nearest imaginary axis

Finding eigenvalues nearest the imaginary axis

- Now assume special case:

$$Ax = (\gamma + \lambda)Bx \quad , \gamma \in \mathbb{R}, \lambda \in i\mathbb{R}$$

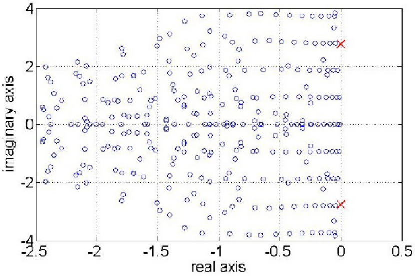
- Computing eigenvalues nearest the imaginary axis
- The method is greatly simplified since $M = B$
  - When Arnoldi is used as Lyapunov solver, Lyapunov inverse iteration corresponds to *implicitly restarted Arnoldi* [M. & Vandebril 2012]
  - When rational Krylov is used with optimal pole selection, the method corresponds to *rational Krylov* with implicit restart [M. 2016] (Close to IRKA for model reduction)



([Beckerman 2012])

Numerical example: driven cavity

Critical Reynolds number is Re $= 7929$
Solve the problem for Re $= 7800$.



k	p	restarts	number of eigenvalues
100	40	2	12
80	40	3	12
60	40	4	12
60	20	5	12
40	20	9	12
20	10	19	7

Conclusions

- Solving parameterized eigenvalue problems is an old problem
- but new ideas are coming up:
  - Jacobi-Davidson method
  - Lyapunov (Sylvester) inverse iteration
- Tests with true problems (Navier-Stokes) are done: nice results.

Bibliography I

H. Elman, K. Meerbergen, A. Spence, and M. Wu.
Lyapunov inverse iteration for identifying Hopf bifurcations in models of incompressible flow.
SIAM J. Sci. Comput., 34(3):A1584–A1606, 2012.

S. Güttel, R. Van Beeumen, K. Meerbergen, and W. Michiels.
NLEIGS: A class of fully rational Krylov methods for nonlinear eigenvalue problems.
SIAM J. Sci. Comput., 36(6):A2842–A2864, 2014.

M. E. Hochstenbach, T. Kosir, and B. Plestenjak.
A Jacobi–Davidson type method for the two-parameter eigenvalue problem.
SIAM J. Matrix Anal. Appl., 26(2):477–497, 2005.

E. Jarlebring, K. Meerbergen, and W. Michiels.
An Arnoldi like method for the delay eigenvalue problem.
SIAM J. Sci. Comput., 32(6):3278–3300, 2010.

Bibliography II

P. Lietaert, K. Meerbergen, J. Perez, and B. Vandereycken.
Automatic rational approximation and linearization of nonlinear eigenvalue problems.
Technical report, 2017.
In preparation.

P. Lietaert, K. Meerbergen, and F. Tisseur.
Compact two-sided krylov metods for nonlinear eigenvalue problems.
Technical Report TW681, KULeuven, Departement of Computer Science, 2017.

K. Meerbergen and A. Spence.
Shift-and-invert iteration for purely imaginary eigenvalues with application to the detection of Hopf bifurcations in large scale problems.
SIAM J. Matrix Anal. and Applic., 31(4):1463–1482, 2010.

R. Van Beeumen, K. Meerbergen, and W. Michiels.
Compact rational Krylov methods for nonlinear eigenvalue problems.
SIAM J. Matrix Anal. and Applic., 36(2):820–838, 2015.