The Computation of Purely Imaginary Eigenvalues with Application to the Detection of Hopf Bifurcations in Large Scale Problems

Karl Meerbergen
(Joint work with Alastair Spence)

K.U. Leuven

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Outline

1. Motivation
2. Three eigenvalue problems
3. Inverse iteration
4. Inexact inverse iteration
5. Numerical example

Detection of Hopf bifurcations

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

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

- 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 λ so that steady state correspond to a Hopf bifurcation

Detection of Hopf bifurcations

- Popular method: linearized stability analysis

$$A(\lambda)x = \mu M x$$

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

Detection of Hopf bifurcations

- We have the following set-up of the problem:
  - Assume $\lambda = 0$ corresponds to a stable steady state: eigenvalues of $A(0)x = \mu Mx$ have negative real parts.
  - We want to compute the Hopf point nearest $\lambda = 0$.
  - Since A is stable, checking the first pair of imaginary eigenvalues as a function of λ is what we need.
- Well studied problem in the literature, e.g. [Govaerts, 2000]
- Detection of unstable branches by transition of real eigenvalues through the origin is an easy problem to solve:
  Find λ, x so that $A(\lambda)x = 0$

General form of the eigenvalue problem

- For a system of nonlinear ODE's, A depends on the eigenvalue and the steady state vector.
  - $A(\lambda)$: for every new λ, a steady state computation is required
  - $A(\lambda)$ is the Jacobian matrix
- In most cases μ is a linear or quadratic eigenvalue
- In many cases λ is linear
- In this talk, we compute 'starting values' for λ for the non-linear ODE.

Bi-alternate product

- Small problems [Guckerheimer et al. 1993, 1997]
- Bi-alternate product:

$$\frac{1}{2}(A(\lambda) \otimes M + M \otimes A(\lambda))$$

  has a pair of zero eigenvalues when $A(\lambda)$ has a pair of purely imaginary eigenvalues.
- Similar ideas were used by [Gu, Mengi, Overton, Xia, Zhu, 2006] to estimate the distance to controllability
- And by [Michiels & Niculescu 2007], [Jarlebring 2008] for determining critical delays
- No exploitation of structure in the eigenvectors

Three eigenvalue problems

Connection between three eigenvalue problems:

PEVP $A(\lambda)x = \mu Mx$

KEVP Kronecker eigenvalue problem (bialternate product)

LEVP Lyapunov eigenvalue problem

Two parameter eigenvalue problem

- Given x en μ so that $A(\lambda)x = \mu Mx$ with μ purely imaginary.
- Then

$$A(\lambda)\bar{x} = -\mu M\bar{x}$$

- and by bringing them together

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

Two parameter eigenvalue problem

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

- In the linear case $A(\lambda) = A_0 + \lambda A_1$:

$$A_0x + \lambda A_1x - \mu Mx = 0$$
$$A_0\bar{x} + \lambda A_1\bar{x} + \mu M\bar{x} = 0$$

This a is two-parameter eigenvalue problem

Two parameter eigenvalue problem

- Solution of the two parameter eigenvalue problem by Jacobi-Davidson style methods [Hochstenbach, Kosir, Plestenjak 2005]
- This method starts from guesses of λ and μ
- For λ, we can use $\lambda = 0$, since we are looking for the smallest λ.
- A good starting guess of μ is *not* so easy to find;
- from experience in other contexts, we know it is a hard problem: a wrong selection may produce a wrong λ.
- Therefore, we want to propose a method that only needs to select λ

Kronecker Eigenvalue Problem (KEVP)

- Observation: if

$$A(\lambda)x = \mu Mx \tag{1}$$

  then for purely imaginary μ:

$$A(\lambda)\bar{x} = -\mu M\bar{x}$$

- and

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

  Proof: from(1) and its conjugation:

$$\begin{aligned} A(\lambda)x \otimes M\bar{x} + Mx \otimes A(\lambda)\bar{x} &= 0 \\ \mu Mx \otimes M\bar{x} - Mx \otimes \mu M\bar{x} &= 0 \end{aligned}$$

- $x \otimes \bar{x}$ is an eigenvector of $(A(\lambda) \otimes M + M \otimes A(\lambda))z = 0$

Spectral properties KEVP

One-to-one correspondance between eigenvalues of (PEVP) and (KEVP):

PEVP		KEVP	
$A(\lambda)x = 0$	$\Leftrightarrow$	$x \otimes x$	simple eigenvalue λ
$\left.\begin{array}{rcl} A(\lambda)x_1 &=& \mu_1 x_1 \\ A(\lambda)x_2 &=& \mu_2 x_2 \\ \mu_1 + \mu_2 &=& 0 \end{array}\right\}$	$\Leftrightarrow$	$x_1 \otimes x_2$ and $x_2 \otimes x_1$	double eigenvalue λ

Since $A(\lambda)$ and M are real, $\mu_{1,2}$ are real or purely imaginary.

Example

Let

$$A(\lambda) = \begin{bmatrix} 2+\lambda & -1 & \\ 1 & 2+\lambda & \\ & & 3 \end{bmatrix} \qquad M = I \ .$$

The eigenvalues of (KEVP) are

- $\lambda = -2$ (double eigenvalue), $\mu = \pm i$
- $\lambda = -2 + i$ (double eigenvalue), $\mu = 2i, i$
- $\lambda = -2 - i$ (double eigenvalue)
- $\lambda = \infty$

Eigenvectors associated with $\lambda = -2$ are $(1, -i, 0) \otimes (1, i, 0)$ and $(1, i, 0) \otimes (1, -i, 0)$.

Lyapunov eigenvalue problem (LEVP)

- From $(A \otimes M + M \otimes A)z = 0$
- to LEVP:

$$A(\lambda)ZM^T + MZA(\lambda)^T = 0$$

with $\mathrm{vec}(Z) = z$

By transposing:

$$A(\lambda)Z^T M^T + MZ^T A(\lambda)^T = 0$$

Suggests for double semi-simple eigenvalues:

- One symmetric 'eigenvector' $Z = Z^T$
- One antisymmetric 'eigenvector' $Z = -Z^T$

Lyapunov eigenvalue problem

(LEVP) has unique symmetric eigenvectors Z:

$$A(\lambda)x = 0 \quad \Leftrightarrow \quad xx^T \quad \text{simple eigenvalue}$$

$$\left.\begin{array}{rcc} A(\lambda)x_1 & = & \mu x_1 \\ A(\lambda)x_2 & = & -\mu x_2 \\ \mu & & \text{real} \end{array}\right\} \quad \Leftrightarrow \quad x_1x_2^T + x_2x_1^T \quad \text{double eigenvalue}$$

$$\left.\begin{array}{rcc} A(\lambda)x & = & \mu x \\ A(\lambda)\bar{x} & = & -\mu \bar{x} \\ \mu & & \text{imaginary} \end{array}\right\} \quad \Leftrightarrow \quad xx^H + \bar{x}x^T \quad \text{double eigenvalue}$$

Symmetric Z is unique up to a scalar factor

Lyapunov eigenvalue problem

(LEVP) has anti-symmetric eigenvectors Z:

$$\left.\begin{array}{rcc} A(\lambda)x_1 & = & \mu x_1 \\ A(\lambda)x_2 & = & -\mu x_2 \\ \mu & & \text{real} \end{array}\right\} \quad \Leftrightarrow \quad x_1 x_2^T - x_2 \otimes x_1 \quad \text{double eigenvalue}$$

$$\left.\begin{array}{rcc} A(\lambda)x & = & \mu x \\ A(\lambda)\bar{x} & = & -\mu \bar{x} \\ \mu & & \text{imaginary} \end{array}\right\} \quad \Leftrightarrow \quad x x^H - \bar{x} \otimes x^T \quad \text{double eigenvalue}$$

Important point: anti-symmetric Z is unique up to a scalar factor

Kronecker eigenvalue problem

- Solution of $A(\lambda) \otimes Mz + M \otimes A(\lambda)z = 0$
- Look at the linearized situation $A = A_0 + \lambda A_1$:

$$(A_0 \otimes M + M \otimes A_0)z = -\lambda(A_1 \otimes M + M \otimes A_1)z$$

- Inverse iteration:
  1. Solve y_{k+1} from $(A_0 \otimes M + M \otimes A_0)y_{k+1} = (A_1 \otimes M + M \otimes A_1^T)z_k$
  2. Normalize $z_{k+1} = y_{k+1}/\|y_{k+1}\|_2$
- Working with n^2-vectors is not practical

Lyapunov eigenvalue problem

- Solution of $A(\lambda)ZM^T + MZA(\lambda)^T = 0$
- Look at the linearized situation $A = A_0 + \lambda A_1$:

$$A_0 ZM^T + MZA_0^T = -\lambda(A_1 ZM^T + MZA_1^T)$$

- Inverse iteration:
  1. Solve Y_{k+1} from $A_0 Y_{k+1} M^T + M Y_{k+1} A_0^T = A_1 Z_k M^T + M Z_k A_1^T$
  2. Normalize $Z_{k+1} = Y_{k+1}/\|Y_{k+1}\|_F$
- If Z_0 is symmetric, all Z_k, $k > 0$, are symmetric.
- Solution of Lyapunov equation on each iteration.
- Is equivalent to inverse iteration on (KEVP)

Lyapunov solvers

- Solve Z from
$$SZ + ZS^T = -bb^T$$
- Unique solution when S is stable.
- Working with full matrices is impractical for large problems
- Approximate Lyapunov solution by a low rank matrix VDV^T with $V^TV = I$.
- Krylov methods (extended Krylov methods) [Many papers]
- ADI type, Smith type method [Many papers]
- We use Krylov methods, i.e.
$$Z = V_k D_k V_k^T$$
with V_k Krylov vectors and $k \ll n$.

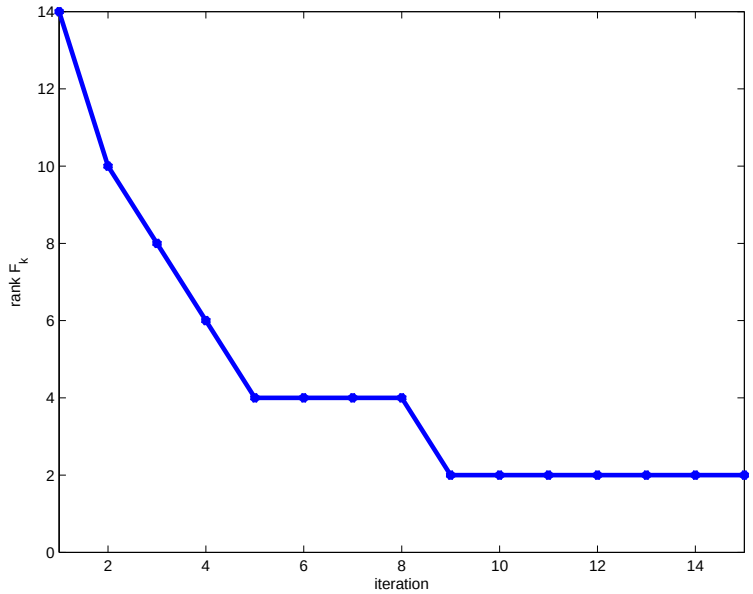
Inverse iteration for LEVP

Difficulties:

- Lyapunov solvers assume a low rank right-hand side for efficient computation.
  We will add a projection step to enforce rank 2 eigenvector iterates
- Use of inexact Lyapunov solvers: inexact inverse iteration
  How accurately do we have to solve the Lyapunov equation?

Enforcing rank 2 iterates

- The right hand side is $F_k = A_1 Z_k M^T + M Z_k A_1^T$.



- F_k is not necessarily of very low rank.
- For large k, Z_k will be of small numerical rank (1 or 2), and thus, F_k has rank 2 or 4.

Enforcing rank 2 iterates (KEVP)

- Range($V_k \otimes V_k$) is a k^2 dimensional subspace containing $z_k = \mathrm{vec}(Z_k)$
- Project (KEVP) onto $V_k \otimes V_k$
- Then we obtain a 'better' Ritz pair
- with low rank Ritz vector (1 or 2)
- In practice:
  - Let $y_k = V_k \otimes V_k \hat{y}$
  - Projection of (KEVP) on $V_k \otimes V_k$:
    Compute eigenvalues nearest 0 of

$$(\widehat{A}_0 \otimes \widehat{M} + \widehat{M} \otimes \widehat{A}_0)\widehat{y} = -\lambda(\widehat{A}_1 \otimes \widehat{M} + \widehat{M} \otimes \widehat{A}_1)\widehat{y}$$

    with

$$\widehat{A}_0 = V_k A_0 V_k \quad \widehat{A}_1 = V_k A_1 V_k \quad \widehat{M} = V_k^T M V_k$$

Enforcing rank 2 iterates (LEVP)

- Projection step:
  - Let $Y_k = V_k \widehat{Y} V_k^T$
  - Projection of (LEVP):
    Compute eigenvalues nearest 0 of

$$\widehat{A}_0 \widehat{Y} \widehat{M}^T + \widehat{M} \widehat{Y} \widehat{A}_0^T = -\lambda(\widehat{A}_1 \widehat{Y} \widehat{M}^T + \widehat{M} \widehat{Y} \widehat{A}_1^T)$$

    with

$$\widehat{A}_0 = V_k A_0 V_k \quad \widehat{A}_1 = V_k A_1 V_k \quad \widehat{M} = V_k^T M V_k$$

- $\widehat{Y}$ has rank 1 or 2.
- $Y_k = V_k \widehat{Y} V_k^T$ has the same rank as $\widehat{Y}$

Inverse iteration for small scale LEVP

- Compute eigenvalues nearest 0 of the $k \times k$ LEVP

$$\widehat{A}_0 \widehat{Y} \widehat{M}^T + \widehat{M} \widehat{Y} \widehat{A}_0^T = -\lambda(\widehat{A}_1 \widehat{Y} \widehat{M}^T + \widehat{M} \widehat{Y} \widehat{A}_1^T)$$

- This is problem of order k^2.
- The QR method can be expensive, e.g. $k = 50$, $k^2 = 2500$
- We use inverse iteration using full matrices, with Bartels-Stewart as Lyapunov solver [Bartels & Stewart 1972] [Golub, Nash & Van Loan 1979] [Hammarling 1982].

Inexact inverse iteration

- The Lyapunov equation is not solved exactly
- So, we have inexact inverse iteration
- Many papers on inexact inverse iteration, with similar conclusions.
  [Lehoucq and M. 1998], [Freitag & Spence], [Hochstenbach & Notay 2009]

Inexact inverse iteration for standard eigenproblem

- Standard eigenvalue problem: $Ax = \lambda x$
- Inexact inversion:

$$Ay_{k+1} = x_k + s_k$$

  with s_k the linear system residual
- A good starting vector is $\lambda_k^{-1} x_k$
- If $r_k = Ax_k - \lambda_k x_k$, then make sure that $\|s_k\| \leq \tau \|r_k\|$ with $\tau < 1$.
- This can be achieved with a constant number of iterations of a Krylov method on A with starting vector x_k.

Inexact inverse iteration for (LEVP)

- Use Krylov method for

$$A_0 Y_{k+1} M^T + M Y_{k+1} A_0^T = M Z_k A_1^T + A_1 Z_k M^T$$

- With $Z_k = V_k D_k V_k^T$, the starting vectors of the Krylov method are $[MV_k, A_1 V_k]$
- If we have two Ritz vectors x_1 and x_2 with residuals r_1 and r_2:

$$r_j = A(\lambda_j)x_j + \mu M x_j$$

- then the starting vectors of the Krylov method contain $x_1 - r_1$ and $x_2 - r_2$.
- We have a similar situation as for the standard eigenvalue problem.

Numerical example

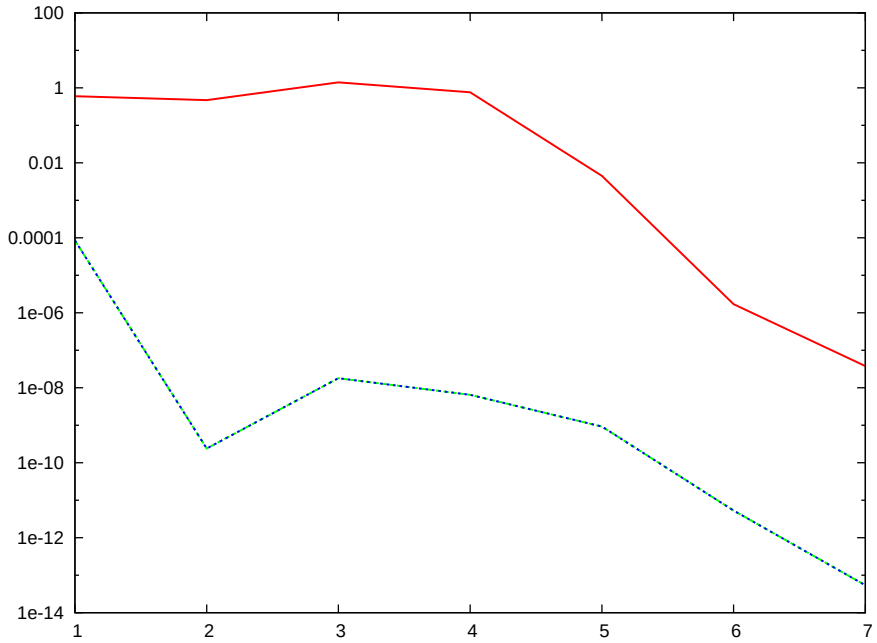
- Olmstead equation

$$\begin{aligned} \frac{\partial u}{\partial t} &= (1-C)\frac{\partial^2 v}{\partial X^2} + C\frac{\partial^2 u}{\partial X^2} + Ru - u^3 \\ B\frac{\partial v}{\partial t} &= u - v \end{aligned}$$

- Linearization and spatial discretization: $(A_0 + \lambda A_1)x = \mu x$ with $\lambda = R$
- $n = 20,000$

Numerical example

- Krylov space of dimension 20.



red $= \|A(\lambda)x - \mu Mx\|_2$
blue = Lyapunov residual norm

Non-linear eigenvalue problems

- For polynomial eigenvalue problems, similar ideas can be used, using a detour via a Companion linearization
- Residual inverse iteration for truly non-linear problems