Lecture 2: Numerical Methods for Hopf bifurcations and periodic orbits in large systems

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1 Introduction

2 Calculation of Hopf points

3 Hopf detection using bifurcation theory

4 Hopf detection using Complex Analysis

5 Hopf detection using the Cayley Transform

6 Stable and unstable periodic orbits
Outline

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2. Calculation of Hopf points
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5. Hopf detection using the Cayley Transform
6. Stable and unstable periodic orbits
Recap and plan for today

- **Lecture 1:**
  1. Compute paths of $F(x, \lambda) = 0$ using pseudo-arclength
  2. Detect singular points $\text{Det}(F_x(x, \lambda)) = 0$
  3. Compute paths of singular points in two-parameter problems
  4. Bordered systems
  5. 4-6 cell interchange in the Taylor problem

- **Lecture 2:**
  - Accurate calculation of Hopf points
  - Detection of Hopf bifurcations (find pure imaginary eigenvalues in a large sparse parameter-dependent matrix)
    1. Bifurcation theory
    2. Complex analysis
    3. Cayley transform
  - Stable and unstable periodic orbits
Lecture 1: Compute singular points

- Seek \((x, \lambda)\) such that \(F_x(x, \lambda)\) is singular
- Consider
  \[
  \begin{bmatrix}
  F_x(x, \lambda) & F_\lambda(x, \lambda) \\
  c^T & d
  \end{bmatrix}
  \begin{bmatrix}
  * \\
  g
  \end{bmatrix}
  =
  \begin{bmatrix}
  0 \\
  1
  \end{bmatrix}
  \]
- \(\text{Det}(F_x) = 0 \iff g = 0\).
- Accurate calculation: Consider the pair
  \[
  F(x, \lambda) = 0, \quad g(x, \lambda) = 0
  \]
- Newton’s Method:
  \[
  \begin{bmatrix}
  F_x(x, \lambda) & F_\lambda(x, \lambda) \\
  g_x(x, \lambda)^T & g_\lambda(x, \lambda)
  \end{bmatrix}
  \begin{bmatrix}
  \Delta x \\
  \Delta \lambda
  \end{bmatrix}
  =
  -
  \begin{bmatrix}
  F \\
  g
  \end{bmatrix}
  \]
- System nonsingular if \(\frac{d}{dt} \mu \neq 0\) at singular point
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Accurate calculation of Hopf points

- Assume \( A(\lambda) = F_x(x, \lambda) \) is real and nonsingular
- At Hopf point: \( A(\lambda) \) has eigenvalues \( \pm i\omega \)
- \( \text{Rank}(A(\lambda)^2 + \omega^2 I) = n - 2 \)
Accurate calculation of Hopf points

- Assume $A(\lambda) = F_x(x, \lambda)$ is real and nonsingular
- At Hopf point: $A(\lambda)$ has eigenvalues $\pm i\omega$
- $\text{Rank}(A(\lambda)^2 + \omega^2 I) = n - 2$
- Calculate Hopf point using 2-bordered matrix: set up

$$F(x, \lambda) = 0, \quad g(x, \lambda, \omega) = 0, \quad h(x, \lambda, \omega) = 0$$

where

$$\begin{bmatrix}
A(\lambda)^2 + \omega^2 I & B \\
C^T & D
\end{bmatrix}
\begin{bmatrix}
\ast \\
g \\
h
\end{bmatrix}
= 
\begin{bmatrix}
0 \\
r_1 \\
r_2
\end{bmatrix}$$

- Newton system, $(n + 2) \times (n + 2)$, needs $g_x, g_\lambda, g_\omega, h_x, \ldots$
- Block version of (D)+iterative refinement on (C)
- 2-bordered matrix is nonsingular if complex pair cross imaginary axis “smoothly”
Hopf continued

- $A(\lambda) = F_x(x, \lambda)$
- If you don’t want to form $A(\lambda)^2$: split complex eigenvector/eigenvalue into Real and Imaginary parts and work with $(2n + 2) \times (2n + 2)$ matrices involving $A(\lambda)$
- Extensions for N-S: $A(\lambda)\phi = \mu B\phi$
- **BUT**: Whatever system is used, accurate estimates for $\lambda$ and $\omega$ are needed
- Compute paths of Hopf points in 2-parameter problems (3-bordered matrices)
- Summary of methods: Govaerts (2000)
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Bifurcation Theory: Takens-Bogdanov (TB) point

At a TB point, $F_x$ has a 2-dim Jordan block, i.e. \[
\begin{bmatrix}
0 & 1 \\
0 & 0
\end{bmatrix}.
\]
A typical picture is:
“Organising Centre” Algorithm

- Two parameter problem $F(x, \lambda, \alpha) = 0$
- Fix $\alpha$. Compute a Turning point in $(x, \lambda)$ (**Easy**). Remember:

\[
F_x \phi = 0, \quad (F_x)^T \psi = 0
\]

- For the 2-parameter problem: Compute path of Turning points looking for $\psi^T \phi = 0$ (TB point) (**Easy**)
- Jump onto path of Hopf points (symmetry-breaking) (**Easy**)
- Compute path of Hopf points (pseudo-arclength) (**Easy**)
- In parameter space the paths of Hopf and Turning points are **tangential** at TB
5 cell anomalous flows in the Taylor Problem

Figure: Two different 5-cell flows
5-cell flows experimental results

**Figure:** parameter space plots of 5-cell flows
5-cell flows numerical results (Anson)

**Figure:** parameter space plots of 5-cell flows
“Organising Centre” approach

Figure: 5-cell flows: Sequence of Bifurcation diagrams as aspect ratio changes

This understanding wouldn’t be possible without the numerical results
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The “idea”: Govaerts/Spence (1996)

**Figure**: For each point on $F(x, \lambda) = 0$ can we calculate the number of eigenvalues in the unstable half plane?

**Why Nice?**

(a) Seek an integer, and (b) Estimate for $\text{Im}(\mu)$ not needed.
**Complex Analysis**

**Winding number**

If \( g(z) \) is analytic in \( \Gamma \)

\[
N - P = \frac{1}{2\pi} \left[ \arg g(z) \right]_{\Gamma} = \text{Winding Number} = W(g)
\]

**Contour for real matrices**

**Algorithm**

Complex Analysis

Winding number

If $g(z)$ is analytic in $\Gamma$

\[ N - P = \frac{1}{2\pi}[\arg g(z)]_{\Gamma} \]

= Winding Number

= $W(g)$

Contour for real matrices

Algorithm

- If $g$ changes so that a real pole crosses Left to Right, $W(g)$ decreases by $\pi$. (real zero crosses L to R then $W(g)$ increases)
- If $g$ changes so that a complex pole crosses Left to Right, $W(g)$ decreases by $2\pi$
Complex Analysis

Winding number

If $g(z)$ is analytic in $\Gamma$

$$N - P = \frac{1}{2\pi} \arg g(z)|_{\Gamma}$$

= Winding Number

= $W(g)$

Contour for real matrices

Algorithm

- If $g$ changes so that a real pole crosses Left to Right, $W(g)$ decreases by $\pi$. (real zero crosses L to R then $W(g)$ increases)
- If $g$ changes so that a complex pole crosses Left to Right, $W(g)$ decreases by $2\pi$
- Need to evaluate $g(iy))$ on $\Gamma$
How to choose $g(z)$?

- Don’t choose $g(z) = \text{Det}(A(\lambda) - zI)$
- $g(z) = c^T (A(\lambda) - zI)^{-1}b$
- Schur complement of $M = \begin{bmatrix} A(\lambda) - zI & b \\ c^T & 0 \end{bmatrix}$
- poles are eigenvalues of $A(\lambda)$; zeros depend on choices of $b$ and $c$. Choose $b$ and $c$ so that the zeros “cancel” the poles to keep $W(g)$ “small”
- Need to evaluate $g(iy) = c^T (A(\lambda) - iyI)^{-1}b$ as $y$ moves up Imaginary axis (Ying/Katz algorithm chooses $y$’s)
The Tubular Reactor problem (Govaerts/Spence, 1996)

- Coupled pair of nonlinear parabolic PDEs for Temperature and Concentration
- Scaling: for a complex pole crossing Imag axis $W(g)$ reduces by 4
The Tubular Reactor problem (Govaerts/Spence, 1996)

- Coupled pair of nonlinear parabolic PDEs for Temperature and Concentration
- Scaling: for a complex pole crossing Imag axis $W(g)$ reduces by 4
- Winding numbers for 3 choices of $g$

<table>
<thead>
<tr>
<th>point on path</th>
<th>$W(g_1)$</th>
<th>$W(g_2)$</th>
<th>$W(g_3)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>5</td>
<td>3*</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>5</td>
<td>3</td>
</tr>
<tr>
<td>5</td>
<td>$-1^\dagger$</td>
<td>$1^\dagger$</td>
<td>$-1^\dagger$</td>
</tr>
<tr>
<td>6</td>
<td>$-1$</td>
<td>$3^\ddagger$</td>
<td>$1^\ddagger$</td>
</tr>
</tbody>
</table>

$^* =$ zero of $g_3$

$^\dagger =$ Hopf!

$^\ddagger =$ zero of $g_2$ and $g_3$. 
Final comments on “Winding Number” algorithm

- Govaerts/Spence was “proof of concept”: tested on a “not too difficult” problem
- Work is to evaluate
  \[ g(iy) = c^T(A(\lambda) - iyI)^{-1}b \]
  as \( y \) moves up Imaginary axis
- For PDE matrices - Krylov solvers/model reduction?
- Ideas from yesterday’s lectures by Strakos (scattering amplitude) and Ernst (frequency domain).
- Also: Stoll, Golub, Wathen (2007)
- Note: you choose \( b \) and \( c \)!
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The Cayley Transform

\[ A\phi = \mu B\phi \]

Choose \( \alpha \) and \( \beta \) and form:

\[ C = (A - \alpha B)^{-1}(A - \beta B) \quad \text{The Cayley transform} \]

- As \( \lambda \) varies, if \( \mu \) crosses the line \( \text{Re}(\alpha + \beta)/2 \) then \( \theta \) moves outside the unit ball.

**Figure:** The mapping of \( \mu \) to \( \theta \)
Hopf detection using the Cayley Transform

- Mapping
  \[ \theta = (\mu - \alpha)^{-1}(\mu - \beta) \]

- So \( \beta = -\alpha \) maps left-half plane ("stable") into unit circle

- Algorithm: At each point on \( F(x, \lambda) = 0 \):
  1. Choose \( \alpha, \beta \)
  2. Monitor dominant eigenvalues of \( C = (A - \alpha B)^{-1}(A - \beta B) \)

- Don’t need to know \( \text{Im}(\mu) \)

- Successfully computed Hopf bifurcations in Taylor problem and Double-diffusive convection

- BUT: "large" eigenvalues, \( \mu \), "cluster" at \( \theta = 1 \)
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Periodic orbits

**Theory**

- $\dot{x} = F(x, \lambda), \ x(t) \in \mathbb{R}^n$
- $x(0) = x(T), \ T=\text{period}$
- Solution ("flow"): $\phi(x(0), t, \lambda)$
- Periodic: $\phi(x(0), T, \lambda) = x(0)$
- Phase condition: $s(x(0)) = 0$
- Stability: Monodromy matrix

$$\phi_x = \frac{\partial \phi}{\partial x(0)}(x(0), T, \lambda)$$

- $\mu_i \in \sigma(\phi_x)$: Floquet multipliers
- Stability: $|\mu_i| < 1, i = 2 \ldots n$ ($\mu_1 = 1$)
- Monodromy matrix is FULL
Stability of periodic orbits

Loss of stability: multiplier crosses unit circle (e.g. real eigenvalue crosses through -1 then “period-doubling bifurcation”)

If solution is stable just integrate in time: OK if $\mu_i$ not near unit circle

“Integrate in time” is no good for unstable orbits

**Figure:** Plot of Floquet multipliers for a stable periodic orbit
Newton-Picard Method for periodic orbits (Lust et. al.)

- **Unknowns:** initial condition, $x(0)$, and period, $T$, (drop $\lambda$)
- **Fixed point problem + phase condition**

  $$\phi(x(0), T) = x(0), \quad s(x(0)) = 0$$
Newton-Picard Method for periodic orbits (Lust et. al.)

- **Unkowns**: initial condition, $x(0)$, and period, $T$, (drop $\lambda$)
- **Fixed point problem + phase condition**

$$\phi(x(0), T) = x(0), \quad s(x(0)) = 0$$

- **Picard Iteration**: Guess $(x(0), T(0))$ and compute $x(1)(0)$

$$\phi(x(0), T(0)) = x(1)(0)$$
Newton-Picard Method for periodic orbits (Lust et. al.)

- **Unknwons**: initial condition, $x(0)$, and period, $T$, (drop $\lambda$)
- Fixed point problem + phase condition

$$\phi(x(0), T) = x(0), \quad s(x(0)) = 0$$

- **Picard Iteration**: Guess $(x^{(0)}(0), T^{(0)})$ and compute $x^{(1)}(0)$

$$\phi(x^{(0)}(0), T^{(0)}) = x^{(1)}(0)$$

- **Newton’s Method**: Guess $(x^{(0)}(0), T^{(0)})$ and compute corrections

$$\begin{bmatrix}
\phi_x - I & \phi_T \\
 s_x & 0
\end{bmatrix}
\begin{bmatrix}
\Delta x(0) \\
\Delta T
\end{bmatrix}
= -
\begin{bmatrix}
r_1 \\
r_2
\end{bmatrix}$$
Newton-Picard Method for periodic orbits (Lust et. al.)

- **Unkowns:** initial condition, \( x(0) \), and period, \( T \), (drop \( \lambda \))
- **Fixed point problem + phase condition**

\[
\phi(x(0), T) = x(0), \quad s(x(0)) = 0
\]

- **Picard Iteration:** Guess \( (x^{(0)}(0), T^{(0)}) \) and compute \( x^{(1)}(0) \)

\[
\phi(x^{(0)}(0), T^{(0)}) = x^{(1)}(0)
\]

- **Newton’s Method:** Guess \( (x(0)^{(0)}, T^{(0)}) \) and compute corrections

\[
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\phi_x - I & \phi_T \\
s_x & 0
\end{bmatrix}
\begin{bmatrix}
\Delta x(0) \\
\Delta T
\end{bmatrix}
= -
\begin{bmatrix}
r_1 \\
r_2
\end{bmatrix}
\]

- **Newton-Picard Method:** Split \( \mathbb{R}^n \) into “stable” and “unstable” subspaces. Convergence? - **Modified Newton**
  1. Picard on “stable” subspace (large)
  2. Newton on “unstable” subspace (small)
  3. Schroff&Keller: “Recursive Projection Method” - computing stable and unstable steady states using initial value codes
Newton-Picard Method for periodic orbits

Figure: Splitting of Floquet multipliers into “stable” and “unstable” subsets

- Pick $\rho < 1$
- “Stable”: $|\mu_i| < \rho$ (hopefully dimension $\approx n$)
- “Unstable”$: |\mu_i| \geq \rho$ (hopefully dimension very small)
Floquet multipliers for the Brusselator

Figure: Floquet multipliers

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Hopf bifurcations and periodic orbits
Lots of Numerical Linear Algebra!

1. Find (orthogonal) basis for “unstable” space, called $V$
2. Construct projectors onto “unstable” and “stable” spaces
3. need the action of $\phi_x$ on $V$ (implemented by a small number of ODE solves)
4. need to increase /decrease dimension of $V$ as Floquet multipliers enter or leave the “unstable” space
5. need to compute paths of periodic orbits: use pseudo-arclength (bordered matrices)
Conclusions

- An efficient method to roughly “detect” a Hopf bifurcation in large systems is still an open problem.
- Methods exist for accurate calculation once good starting values are known.
- Look again at the winding number algorithm?
- Computation of stable and unstable periodic solutions for discretised PDEs (e.g. Navier-Stokes) is wide open!
- Software:
  1. LOCA “Library of Continuation Algorithms” Sandia (PDEs)
  2. MATCONT “Continuation software in Matlab”: W Govaerts
  3. AUTO