Spectral Inclusion Regions for Bifurcation Analysis

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Outline

Stability of reaction-diffusion systems

Subspace projection and the field of values

Subspace projection and pseudospectral bounds

Conclusions
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Conclusions
Belousov-Zhabotinski reaction

www.pojman.com/NLCD-movies/NLCD-movies.html
Reaction-diffusion models

\[ \frac{\partial u}{\partial t} = D \nabla^2 u + F(u; s) \]

Describes many systems:

- Chemical reactions (like the B-Z reaction)
- Signals in nerves
- Ecological systems
- Phase transitions

See *Chemical Oscillations, Waves, and Turbulence* (Kuramoto).
Stability analysis

Linearize about an equilibrium branch \( u_0(s) \):

\[
\frac{\partial}{\partial t} \delta u = \left( D\nabla^2 + F_u(u_0(s); s) \right) \delta u = J(s) \delta u
\]

- Stable if eigenvalues of \( J(s) \) have negative real part
- When stability changes, have a bifurcation
- Complex eigs cross imaginary axis \( \Rightarrow \) oscillations, a Hopf bifurcation
The Brusselator

- Two-component model of B-Z reaction
- Reaction takes place in a narrow tube of length $L$
- Stable constant equilibrium for small $L$
- Hopf bifurcation at a critical value of $L$
Hopf bifurcation in the Brusselator
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Generally: have (discretized) Jacobian $J(s)$
Want to know when $J(s)$ becomes unstable
Only a few eigenvalues matter for stability analysis
Compute those eigenvalues by continuation
How many eigenvalues do we need?
Subspace projections

\[ JQ = Q \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{bmatrix} \]

- Arnoldi’s method \( \rightarrow \) block Schur form
- \( T_{11} \) is (quasi)-triangular
- \( T_{22} \) is not known explicitly
- Want some assurance that \( T_{22} \) is stable
  - Without computing eigenvalues of \( T_{22} \)!
Spectral inclusion regions

- To show: some (sub)matrix is stable
- Show eigenvalues live in some inclusion region:
  - Field of values
  - Gershgorin disks
  - Pseudospectra
- Show that inclusion region lies in left half-plane
Field of values

\[ \mathcal{F}(A) := \{ x^* Ax : x^* x = 1 \} \]

- Eigenvalues live inside \( \mathcal{F}(A) \)
- (Toeplitz-Hausdorff): \( \mathcal{F}(A) \) is convex
- For \textit{normal} matrices, \( \mathcal{F}(A) = \text{convex hull of } \Lambda(A) \)
- \( \Re(\mathcal{F}(A)) = \mathcal{F}(H(A)) = [\lambda_{\text{min}}(H(A)), \lambda_{\text{max}}(H(A))] \)

Hard to compute \( \mathcal{F}(A) \), easy to estimate the \textit{numerical abscissa}

\[ \omega(A) := \lambda_{\text{max}}(H(A)). \]
Bounding $\mathcal{F}(A)$

$\Re(\lambda) = \lambda_{\text{max}}(H(A))$
Field of values and bifurcation analysis

\[ JQ = Q \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{bmatrix} \]

- Compute some eigenvalues via Arnoldi (for example)
- Estimate \( \omega(T_{22}) = \lambda_{\text{max}}(H(T_{22})) \) via Lanczos
- If estimate is insufficiently negative, compute more eigs
Bound applied to a 2D Brusselator
An Eeyore bound?

Have a growth bound:

\[
\frac{d}{dt} \bigg|_{t=0} \| \exp(tT_{22}) \| = \omega(T_{22})
\]

So if \( \delta u' = J\delta u \), then for any initial conditions,

\[
\frac{d}{dt} \| Q^*_2 \delta u(t) \| \leq 0.
\]

Forcing \( \omega(T_{22}) < 0 \) means \( T_{11} \) accounts for any transient growth as well as any long-term instability.
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Are we there yet?

- Can we miss things between continuation steps?
- What if we don’t have an exact invariant subspace?
- What about finite perturbations to the problem?
- What about large transient growth?
Might want to analyze *pseudospectra* instead of eigenvalues

\[ \Lambda_\epsilon(A) := \{ z \in \mathbb{C} : \sigma_{\min}(A - zI) \leq \epsilon \} \]
\[
= \bigcup_{\|E\| \leq \epsilon} \Lambda(A + E)
\]

- Provide a neat notation for perturbation theorems
- Provides insight into transient effects
- Even more expensive to compute than \( \Lambda(A) \)
Pseudospectra and projections

\[ JQ = Q \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{bmatrix} \]

- \( \Lambda_\epsilon(T_{11}) \subset \Lambda_\epsilon(J) \)
- *Not* generally true that \( \Lambda_\epsilon(J) = \Lambda_\epsilon(T_{11}) \cup \Lambda_\epsilon(T_{22}) \)
- But \( \Lambda_\epsilon(T_{11}) \) sometimes gives tight information...
Schur complement bounds

Partition any matrix $A$ as

$$
A = \begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix}
$$

Then

$$
\Lambda(A) \subset \Lambda(A_{22}) \cup \{\lambda \in \mathbb{C} : B(\lambda) \text{ singular}\}
$$

$$
B(\lambda) = (A_{11} - \lambda I) - A_{12}(A_{22} - \lambda I)^{-1}A_{21}
$$

Idea: separately control the two terms in $B(\lambda)$. 


For any $\epsilon > 0$, define

$$
\Omega_\epsilon := \{ \lambda \in \mathbb{C} : \| A_{12} (A_{22} - \lambda I)^{-1} A_{21} \| > \epsilon \}
$$

$$
\subset \{ \lambda \in \mathbb{C} : \| (A_{22} - \lambda I)^{-1} \|^{-1} > \epsilon^{-1} \| A_{12} \| \| A_{21} \| \}
$$

$$
= \Lambda_{\epsilon^{-1} \| A_{12} \| \| A_{21} \|} (A_{22})
$$

Outside $\Omega_\epsilon$, the Schur complement $B(\lambda)$ is within $\epsilon$ of $A - \lambda I$. 
Schur complement bounds

Use norm bounds to localize singularities of $B(\lambda)$

$$\Lambda(A) \subset \Lambda_\epsilon(A_{11}) \cup \Omega_\epsilon \cup \Lambda(A_{22}),$$

and whenever $\gamma_1 \gamma_2 \geq \|A_{12}\| \|A_{21}\|$, 

$$\Lambda(A) \subset \Lambda_{\gamma_1}(A_{11}) \cup \Lambda_{\gamma_2}(A_{22}).$$

Extends naturally to pseudospectra:

$$\Lambda_\epsilon(A) \subset \Lambda_{\tilde{\gamma}_1 + \epsilon}(A_{11}) \cup \Lambda_{\tilde{\gamma}_2 + \epsilon}(A_{22})$$

$$\tilde{\gamma}_1 \tilde{\gamma}_2 \geq (\|A_{12}\| + \epsilon)(\|A_{21}\| + \epsilon)$$
Define the *pseudospectral abscissa*

\[
\alpha_\epsilon(A) := \max \Re(\Lambda_\epsilon(A)).
\]

The *distance to instability* is the smallest \( \delta > 0 \) such that

\[
\alpha_\delta(A) \geq 0.
\]

Can use our Schur complement bounds to bound the distance to instability.
Bounds on distance to instability

For \( \tilde{\gamma}_1 \tilde{\gamma}_2 \geq (\|A_{12}\| + \epsilon)(\|A_{21}\| + \epsilon) \), have

\[
\alpha_\epsilon(A) \leq \max (\alpha_{\tilde{\gamma}_1 + \epsilon}(A_{11}), \alpha_{\tilde{\gamma}_2 + \epsilon}(A_{22})) \\
\leq \max (\alpha_{\tilde{\gamma}_1 + \epsilon}(A_{11}), \omega(A_{22}) + \tilde{\gamma}_2 + \epsilon).
\]
Bounds on distance to instability

Let

\[ \delta = \text{distance from } A \text{ to instability} \]
\[ \delta_1 = \text{distance from } A_{11} \text{ to instability} \]

Then the Schur complement bounds give us

\[
\left( 1 - \frac{\|A_{12}\| + \delta_1}{\omega(A_{22})} \right)^{-1} \delta_1 \leq \delta \leq \delta_1.
\]
Distance to instability: 1D Brusselator example
Brusselator: Bounds on distance to instability

<table>
<thead>
<tr>
<th>Subspace dimension</th>
<th>Distance to instability</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Lower bound</td>
</tr>
<tr>
<td></td>
<td>Upper bound</td>
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</tbody>
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[Graph showing the relationship between subspace dimension and distance to instability with lower and upper bounds.]
Brusselator: Bounds on distance to instability

![Graph showing the relative difference in bounds vs. subspace dimension. The graph indicates a decreasing trend as the subspace dimension increases.]
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Recap

- Goal was to analyze stability by subspace projections
- Want to ensure the subspace contains everything relevant
- Basic recipe: Schur complement + rough bounds on complementary space
- Same recipe gives bounds on pseudospectra, distance to instability
Conclusion

Some preliminary results:

- Have tried the bounds for small pseudospectral discretizations of Brusselator, some other problems
- Seems to work well for these problems
- Have some idea when the bounds ought to give good information (self-adjoint + relatively compact, not too close to singular perturbation)

Lots of remaining questions:

- Can I do better than Lanczos for estimating $\omega(A_{22})$ (and would it make a difference)?
- Are these bounds useable for step-size control in a bifucation code?
- How useful will these bounds be for large problems?