Spectral Inclusion Regions for Bifurcation Analysis

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Outline

Stability of reaction-diffusion systems

Invariant subspace projection and spectral bounds

Subspace projection and pseudospectral bounds

Conclusions
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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 $\implies$ 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 normal matrices, \( \mathcal{F}(A) = \) convex hull of \( \Lambda(A) \)
- Let \( H(A) := \frac{1}{2}(A + A^*) \); then

\[ \Re(\mathcal{F}(A)) = \mathcal{F}(H(A)) = [\lambda_{\min}(H(A)), \lambda_{\max}(H(A))] \]

Hard to compute \( \mathcal{F}(A) \), easy to estimate the numerical abscissa \( \omega(A) := \lambda_{\max}(H(A)) \).
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:

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

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?
Pseudospectra

Might want to analyze \emph{pseudospectra} instead of eigenvalues

\[ \Lambda_\epsilon(A) := \{ z \in \mathbb{C} : \| (A - zI)^{-1} \| \geq \epsilon^{-1} \} \]
\[ = \{ z \in \mathbb{C} : \sigma_{\text{min}}(A - zI) \leq \epsilon \} \]
\[ = \bigcup_{\|E\| \leq \epsilon} \Lambda(A + E) \]

- Provides a neat notation for perturbation theorems
- Provides insight into transient effects
- Even more expensive to compute than \( \Lambda(A) \)
Generalized pseudospectra

Given $B(z)$, define

$$\Lambda(B) := \{ z \in \mathbb{C} : \| B(z)^{-1} \| = \infty \}$$

$$\Lambda_\epsilon(B) := \{ z \in \mathbb{C} : \| B(z)^{-1} \| \geq \epsilon^{-1} \}$$

$$= \{ z \in \mathbb{C} : \sigma_{\min}(B(z)) \leq \epsilon \}$$

- Gives ordinary pseudospectrum for $B(z) = A - zI$
- $\Lambda_\epsilon(B)$ are nested sets, contain $\Lambda(B)$
- If $B$ is analytic in $z$, then any bounded connected component of $\Lambda_\epsilon(B)$ contains part of $\Lambda(B)$
Generalized pseudospectrum perturbation

Given $B(z)$, define

\[
\Lambda_\epsilon(B) := \{ z \in \mathbb{C} : \|B(z)^{-1}\| \geq \epsilon^{-1} \}
\]
\[
= \{ z \in \mathbb{C} : \sigma_{\min}(B(z)) \leq \epsilon \}
\]

If we also have $E(z)$, then

\[
\sigma_{\min}(B + E) \leq \sigma_{\min}(B) + \|E\|
\]
\[
\Lambda_\epsilon(B + E) \subset \Lambda_{\epsilon + \delta}(B) \cup \Omega_\delta
\]
\[
\Omega_\delta := \{ z : \|E(z)\| > \delta \} 
\]
Generalized pseudospectrum perturbation

For $B(z) = A -zl + E(z)$, boundaries of $\Omega_\delta$, $\Lambda_\epsilon+\delta(A)$, $\Lambda_\epsilon(B)$
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
- Analysis tool: go through a nonlinear eigenvalue problem
Schur complement bounds

Partition any matrix $A$ as

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

Then

$$\Lambda(A) \subset \Lambda(A_{22}) \cup \Lambda(B)$$

$$B(\lambda)^{-1} := \begin{bmatrix} (A - \lambda I)^{-1} \end{bmatrix}_{11}$$

$$B(\lambda) = (A_{11} - \lambda I) - E(\lambda)$$

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

Idea: separately control $A_{11} - \lambda I$ and $E(\lambda)$. 
For any $\epsilon > 0$, define

$$\Omega_\epsilon := \{ \lambda \in \mathbb{C} : \| E(\lambda) \| > \epsilon \}$$

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

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

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

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

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

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

\[
\alpha_{\epsilon}(A) \leq \max \left( \alpha_{\tilde{\gamma}_1 + \epsilon}(A_{11}), \alpha_{\tilde{\gamma}_2 + \epsilon}(A_{22}) \right)
\leq \max \left( \alpha_{\tilde{\gamma}_1 + \epsilon}(A_{11}), \omega(A_{22}) + \tilde{\gamma}_2 + \epsilon \right).
\]
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

\[ \text{dim} = 78 \]
Brusselator: Bounds on distance to instability

![Graph showing bounds on distance to instability](image)

- **Subspace dimension**
- **Distance to instability**
- **Lower bound**
- **Upper bound**
Brusselator: Bounds on distance to instability

![Graph showing the relative difference in bounds against subspace dimension.](image-url)
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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?