Spectral Inclusion Regions for Bifurcation Analysis

D. Bindel

Courant Institute for Mathematical Sciences
New York Univerity

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Outline

Stability of reaction-diffusion systems

Invariant subspace projection and spectral bounds

Subspace projection and pseudospectral bounds

Conclusions

Outline

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 $u_0(s)$:

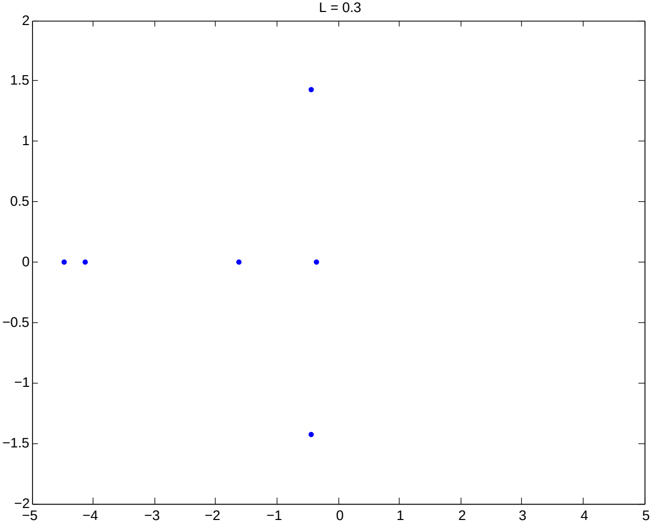
$$\frac{\partial}{\partial t}\delta u = \left(D\nabla^2 + F_u(u_0(s); s)\right)\delta u = J(s)\,\delta u$$

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

The Brusselator

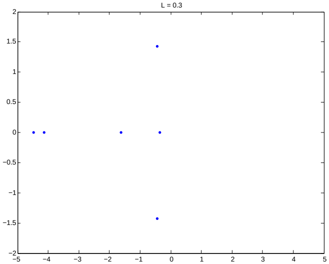
- Two-component model of B-Z reaction
- Reaction takes place in a narrow tube of length L
- Stable constant equilibrium for small L
- Hopf bifurcation at a critical value of L

Hopf bifurcation in the Brusselator



Outline

Subspace projections



- 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

$$\mathcal{F}(A) := \{x^* A x : x^* x = 1\}$$

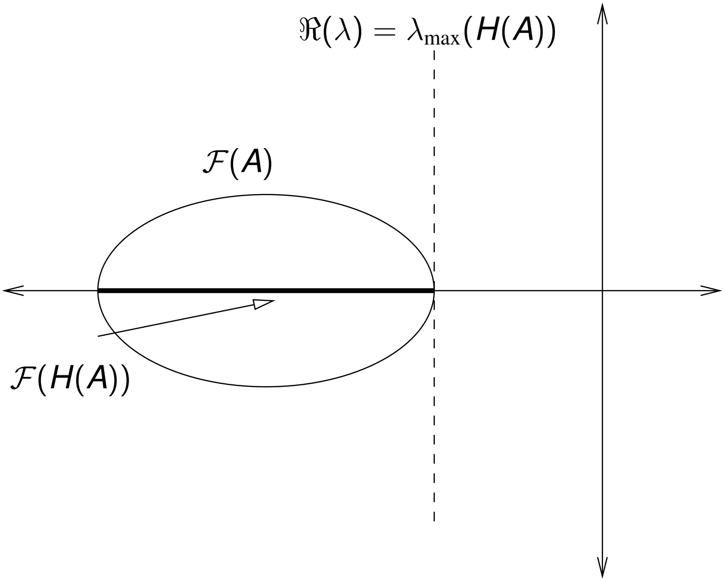
- Eigenvalues live inside $\mathcal{F}(A)$
- (Toeplitz-Hausdorff): $\mathcal{F}(A)$ is convex
- For *normal* matrices, $\mathcal{F}(A) =$ convex hull of $\Lambda(A)$
- Let $H(A) := \frac{1}{2}(A + A^*)$; then

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

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

$$\omega(A) := \lambda_{\max}(H(A)).$$

Bounding $\mathcal{F}(A)$

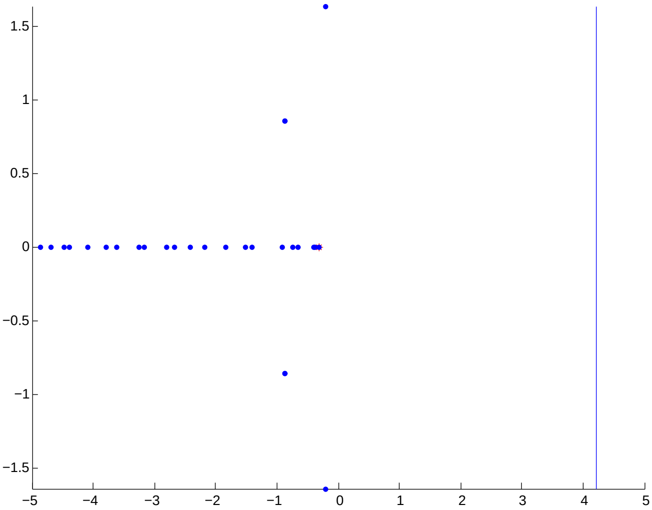


Field of values and bifurcation analysis

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

- Compute some eigenvalues via Arnoldi (for example)
- Estimate $\omega(T_{22}) = \lambda_{\max}(H(T_{22}))$ 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.

Outline

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 *pseudospectra* instead of eigenvalues

$$
\begin{aligned}
\Lambda_\epsilon(A) &:= \{z \in \mathbb{C} : \|(A - zI)^{-1}\| \geq \epsilon^{-1}\} \\
&= \{z \in \mathbb{C} : \sigma_{\min}(A - zI) \leq \epsilon\} \\
&= \bigcup_{\|E\| \leq \epsilon} \Lambda(A + E)
\end{aligned}
$$

- 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

$$\begin{aligned} \Lambda(B) &:= \{z \in \mathbb{C} : \|B(z)^{-1}\| = \infty\} \\ \Lambda_\epsilon(B) &:= \{z \in \mathbb{C} : \|B(z)^{-1}\| \geq \epsilon^{-1}\} \\ &= \{z \in \mathbb{C} : \sigma_{\min}(B(z)) \leq \epsilon\} \end{aligned}$$

- 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

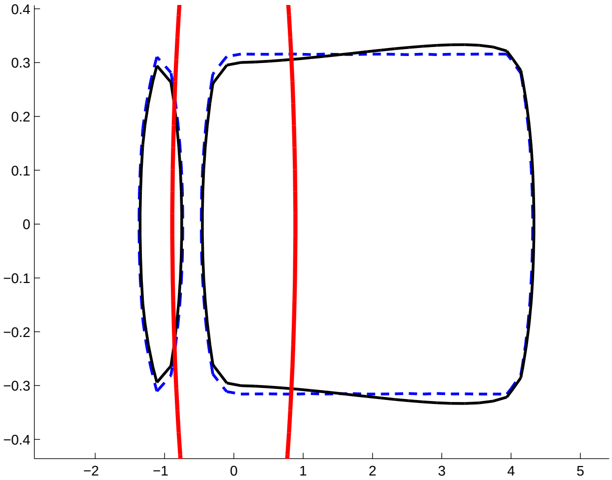
$$\begin{aligned}\Lambda_\epsilon(B) &:= \{z \in \mathbb{C} : \|B(z)^{-1}\| \geq \epsilon^{-1}\} \\ &= \{z \in \mathbb{C} : \sigma_{\min}(B(z)) \leq \epsilon\}\end{aligned}$$

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

$$\begin{aligned}\sigma_{\min}(B+E) &\leq \sigma_{\min}(B) + \|E\| \\ \Lambda_\epsilon(B+E) &\subset \Lambda_{\epsilon+\delta}(B) \cup \Omega_\delta \\ \Omega_\delta &:= \{z : \|E(z)\| > \delta\}\end{aligned}$$

Generalized pseudospectrum perturbation

For $B(z) = A - zI + E(z)$, boundaries of Ω_δ, $\Lambda_{\epsilon+\delta}(A)$, $\Lambda_\epsilon(B)$



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

$$\begin{aligned} \Lambda(A) &\subset \Lambda(A_{22}) \cup \Lambda(B) \\ B(\lambda)^{-1} &:= \left[(A - \lambda I)^{-1}\right]_{11} \\ B(\lambda) &= (A_{11} - \lambda I) - E(\lambda) \\ E(\lambda) &:= A_{12}(A_{22} - \lambda I)^{-1} A_{21} \end{aligned}$$

Idea: separately control $A_{11} - \lambda I$ and $E(\lambda)$.

Schur complement bounds

For any $\epsilon > 0$, define

$$\begin{aligned}
\Omega_\epsilon &:= \{\lambda \in \mathbb{C} : \|E(\lambda)\| > \epsilon\} \\
&= \{\lambda \in \mathbb{C} : \|A_{12}(A_{22} - \lambda I)^{-1} A_{21}\| > \epsilon\} \\
&\subset \{\lambda \in \mathbb{C} : \|(A_{22} - \lambda I)^{-1}\|^{-1} < \epsilon^{-1} \|A_{12}\| \|A_{21}\|\} \\
&= \Lambda_{\epsilon^{-1}\|A_{12}\|\|A_{21}\|}(A_{22})
\end{aligned}$$

Outside Ω_ϵ, the Schur complement $B(\lambda)$ is within ϵ 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:

$$\begin{aligned} \Lambda_\epsilon(A) &\subset \Lambda_{\tilde{\gamma}_1+\epsilon}(A_{11}) \cup \Lambda_{\tilde{\gamma}_2+\epsilon}(A_{22}) \\ \tilde{\gamma}_1 \tilde{\gamma}_2 &\geq (\|A_{12}\| + \epsilon)(\|A_{21}\| + \epsilon) \end{aligned}$$

Application: Distance to instability

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

$$\begin{aligned} \alpha_\epsilon(A) &\leq \max\left(\alpha_{\tilde{\gamma}_1+\epsilon}(A_{11}), \alpha_{\tilde{\gamma}_2+\epsilon}(A_{22})\right) \\ &\leq \max\left(\alpha_{\tilde{\gamma}_1+\epsilon}(A_{11}), \omega(A_{22}) + \tilde{\gamma}_2 + \epsilon\right). \end{aligned}$$

Bounds on distance to instability

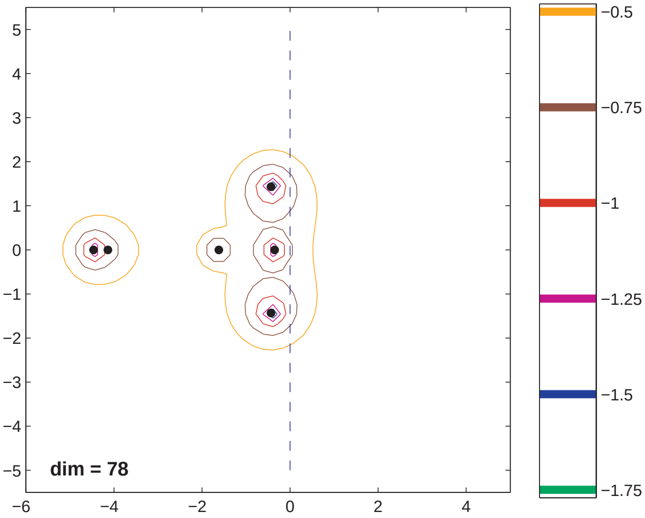
Let

$$\begin{aligned} \delta &= \text{distance from } A \text{ to instability} \\ \delta_1 &= \text{distance from } A_{11} \text{ to instability} \end{aligned}$$

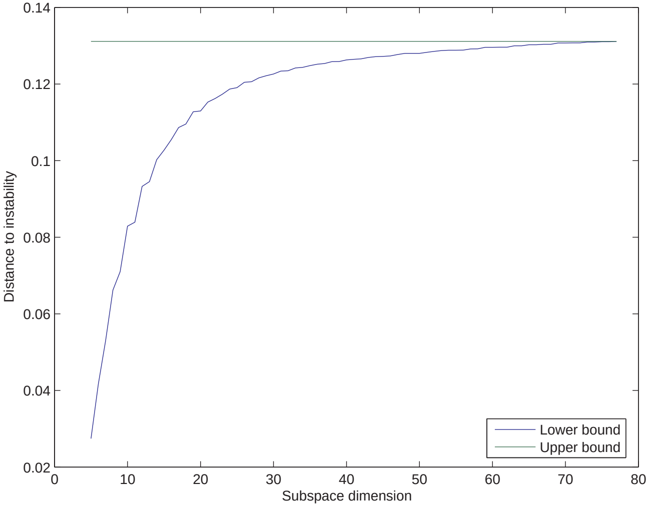
Then the Schur complement bounds give us

$$\left(1 - \frac{\|A_{12}\| + \delta_1}{\omega(A_{22})}\right)^{-1} \delta_1 \leq \delta \leq \delta_1.$$

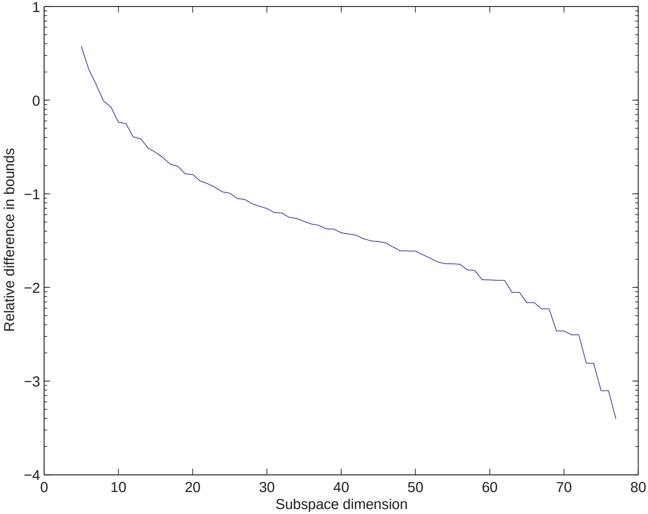
Distance to instability: 1D Brusselator example



Brusselator: Bounds on distance to instability



Brusselator: Bounds on distance to instability



Outline

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?