

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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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 $u_0(s)$:

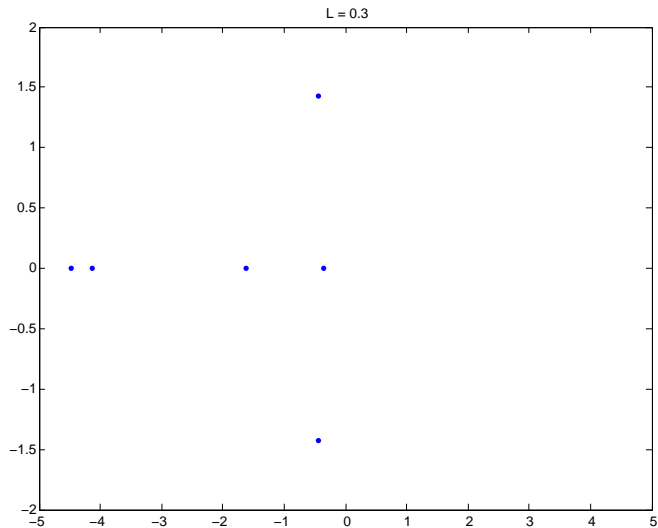
$$\frac{\partial}{\partial t} \delta u = \left(D\nabla^2 + F_u(u_0(s); s) \right) \delta u = J(s) \delta u$$

- ▶ 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

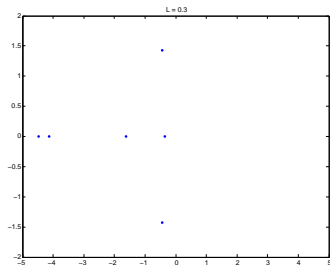
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Subspace projections



- ▶ 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

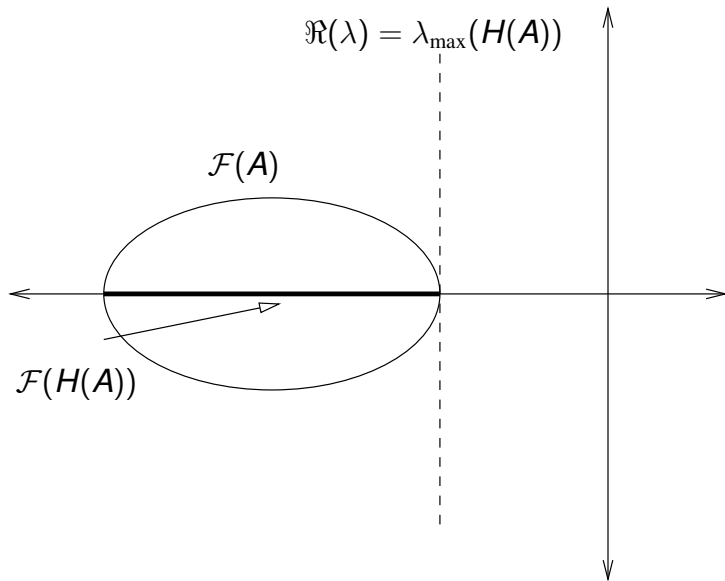
$$\mathcal{F}(A) := \{x^*Ax : x^*x = 1\}$$

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

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

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

Bounding $\mathcal{F}(A)$

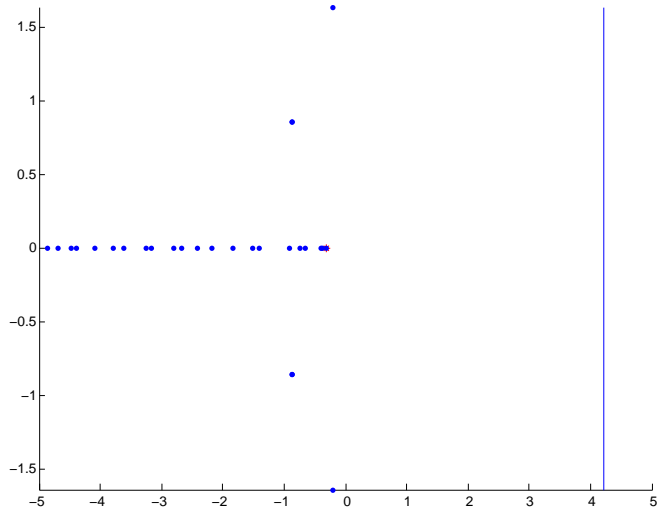


Field of values and bifurcation analysis

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

- ▶ 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.

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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 *pseudospectra* instead of eigenvalues

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

- ▶ 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 $B(\lambda)$.

Schur complement bounds

For any $\epsilon > 0$, define

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

Outside Ω_ϵ , the Schur complement $B(\lambda)$ is within ϵ of $\mathbf{A} - \lambda I$.

Schur complement bounds

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

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

and whenever $\gamma_1 \gamma_2 \geq \|\mathbf{A}_{12}\| \|\mathbf{A}_{21}\|$,

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

Extends naturally to pseudospectra:

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

Application: Distance to instability

Define the *pseudospectral abscissa*

$$\alpha_\epsilon(\mathbf{A}) := \max \Re(\Lambda_\epsilon(\mathbf{A})).$$

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

$$\alpha_\delta(\mathbf{A}) \geq 0.$$

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

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

Bounds on distance to instability

Let

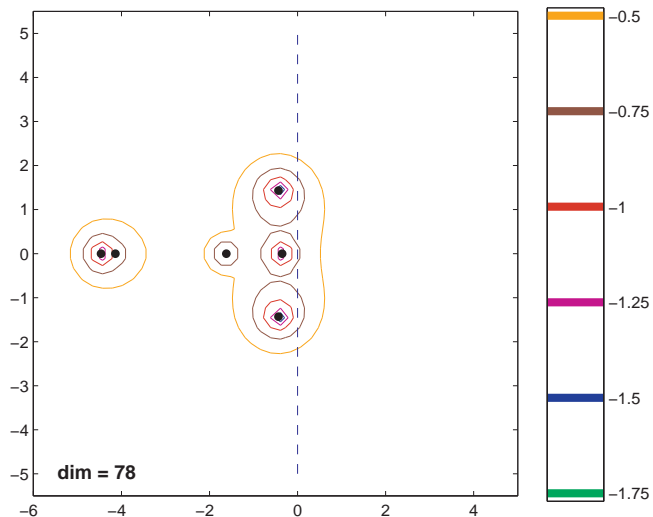
δ = distance from A to instability

δ_1 = distance from A_{11} to instability

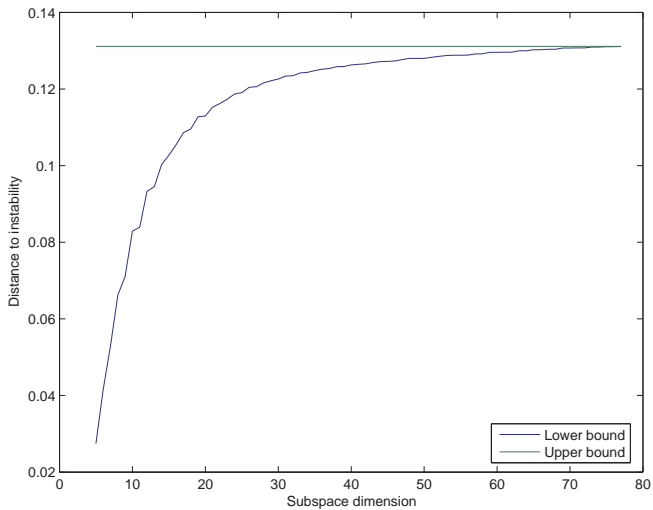
Then the Schur complement bounds give us

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

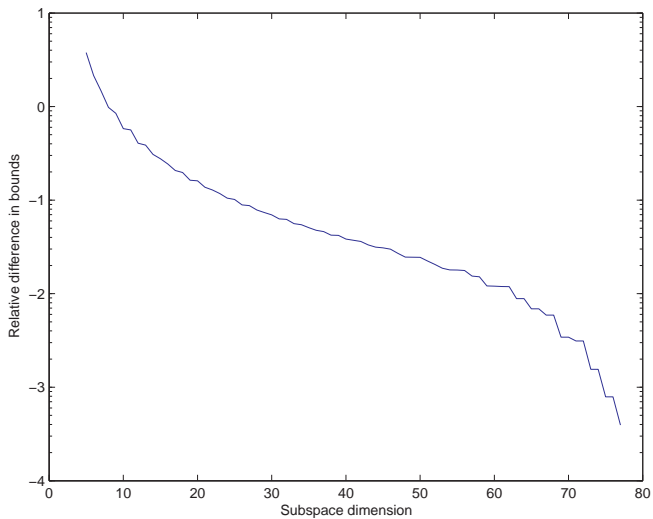
Distance to instability: 1D Brusselator example



Brusselator: Bounds on distance to instability



Brusselator: Bounds on distance to instability



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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 bifurcation code?
- ▶ How useful will these bounds be for large problems?