Outline

- A model reaction-diffusion problem
- Subspace projections and linearized stability
- Estimating fields of values for a termination criterion
- Perturbation theory and pseudospectral estimates
Example: Brusselator

\[ \frac{\partial u}{\partial t} = \frac{D_u}{L^2} \frac{\partial u}{\partial z^2} + f(u, v, \alpha, \beta) \]

\[ \frac{\partial v}{\partial t} = \frac{D_v}{L^2} \frac{\partial v}{\partial z^2} + g(u, v, \alpha, \beta) \]

\[ \alpha = u(0, t) = u(1, t) \]

\[ \beta = v(0, t) = v(1, t) \]

- Simplified 1D reaction-diffusion model
- Unknowns are two chemical concentrations
- Trivial stationary solution: \( u = \alpha \), \( v = \beta / \alpha \)
- When the tube is long enough (\( L \) large enough), get spontaneous waves from an equilibrium mixture
Stability analysis

Linearize about an equilibrium state:

\[
\frac{d}{dt} \begin{bmatrix} \delta u \\ \delta v \end{bmatrix} = \begin{bmatrix} \frac{D_u}{L^2} \frac{\partial^2}{\partial z^2} + f_u & f_v \\ g_u & \frac{D_v}{L^2} \frac{\partial^2}{\partial z^2} + g_v \end{bmatrix} \begin{bmatrix} \delta u \\ \delta v \end{bmatrix} = J \begin{bmatrix} \delta u \\ \delta v \end{bmatrix}
\]

- Stable if eigenvalues of \( J \) have negative real part
- Bifurcation study: change a parameter (\( L \)) and see when stability changes
- Complex eigs cross imaginary axis \( \Rightarrow \) oscillations, a Hopf bifurcation
Generally: have $J(s)$ for some parameter $s$

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 LHP
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*

\[ \omega(A) := \lambda_{\max}(H(A)). \]
\[ \mathcal{R}(\lambda) = \lambda_{\text{max}}(H(A)) \]
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
Have a growth bound:

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

So if \( y' = Jy \), then for any initial conditions,

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

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

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

\[
\Lambda_\epsilon(A) := \{ z : \sigma_{\min}(A - zI) \leq \epsilon \}
\]

\[
= \bigcup_{\|E\| \leq \epsilon} \Lambda(A + E)
\]

- 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...
Partition a matrix $A$ into blocks:

$$A = \begin{bmatrix}
A_{11} & \ldots & A_{1m} \\
\vdots & \ddots & \vdots \\
A_{m1} & \ldots & A_{mm}
\end{bmatrix}$$

Let $R_i := \sum_{j \neq i} \|A_{ij}\|$. Then for any $\epsilon \geq 0$,

$$\bigcup_i \Lambda_{\epsilon - R_i}(A_{ii}) \subset \Lambda_\epsilon(A) \subset \bigcup_i \Lambda_{\epsilon + R_i}(A_{ii})$$

Proof is almost the same as for block Gershgorin (proved in early 1960s).
$Q^* J Q = \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{bmatrix}$

Apply column version of Gershgorin to get:

$\Lambda_\epsilon(J) \subset \Lambda_\epsilon(T_{11}) \cup \Lambda_{\epsilon + \|T_{12}\|}(T_{22})$.

Bound second term:

$\Lambda_{\epsilon + \|T_{12}\|}(T_{22}) \subset \{z : \Re(z) \leq \omega(T_{22}) + \epsilon + \|T_{12}\|\}$

Only useful if $T_{12}$ is not too large.
What if we apply a similarity to block-diagonalize $J$?

$$\Lambda_\epsilon(S^{-1}AS) \subset \Lambda_{\kappa(S)\epsilon}(A)$$

- Similar idea using spectral projectors (§40 in Trefethen and Embree)
- May be annoying to estimate $\kappa(S)$ or norm of a projector
For any $\gamma > 0$, define

$$G = \{ z : \Re(z) < \omega(T_{22}) + \gamma + \epsilon \}.$$  

Then

$$\Lambda_\epsilon(T) \subset G \cup \Lambda_\epsilon(\|T_{12}\|+\epsilon)/\gamma(T_{11}).$$

- Only uses $\omega(T_{22})$ (which we can estimate)
- Bound gets tighter the farther right we go in $\mathbb{C}$
- Haven’t tested it out in computations
Idea of proof

If $\hat{T} - \lambda I = T + E - \lambda I$ is singular, then either
- $\hat{T}_{22} - \lambda I$ is singular, or
- $\hat{T}_{11} - \hat{T}_{12}(\hat{T}_{22} - \lambda I)^{-1}E_{21}$ singular

Now use

$$\sigma_{\min}(T_{22} - \lambda I) \geq \Re(\lambda) - \omega(T_{22})$$

and some norm bounds.

Extends readily to case of an approximate invariant subspace.
Conclusions?

Have a few promising bounds for calculating stability from Arnoldi projections, but:

- Have only tried the spectral bounds (on two examples)
- Small pseudospectral discretizations for initial trials

Some remaining questions:

- Can I do better than Lanczos for estimating $\omega(T_{22})$?
  - And would it make any difference?
- Are these bounds useful for step size control in CIS?
- For what classes of problems does this work well?
  - Probably not singular perturbations (small diffusion)