Inclusion Regions for Bifurcation Analysis

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Outline

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

Belousov-Zhabotinski reaction

www.pojman.com/NLCD-movies/NLCD-movies.html

Example: Brusselator

$$
\begin{aligned}
\frac{\partial u}{\partial t} &= \frac{D_u}{L^2}\frac{\partial u}{\partial z^2} + f(u, v, \alpha, \beta) \\
\frac{\partial v}{\partial t} &= \frac{D_v}{L^2}\frac{\partial v}{\partial z^2} + g(u, v, \alpha, \beta) \\
\alpha &= u(0, t) = u(1, t) \\
\frac{\beta}{\alpha} &= v(0, t) = v(1, t)
\end{aligned}
$$

- 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

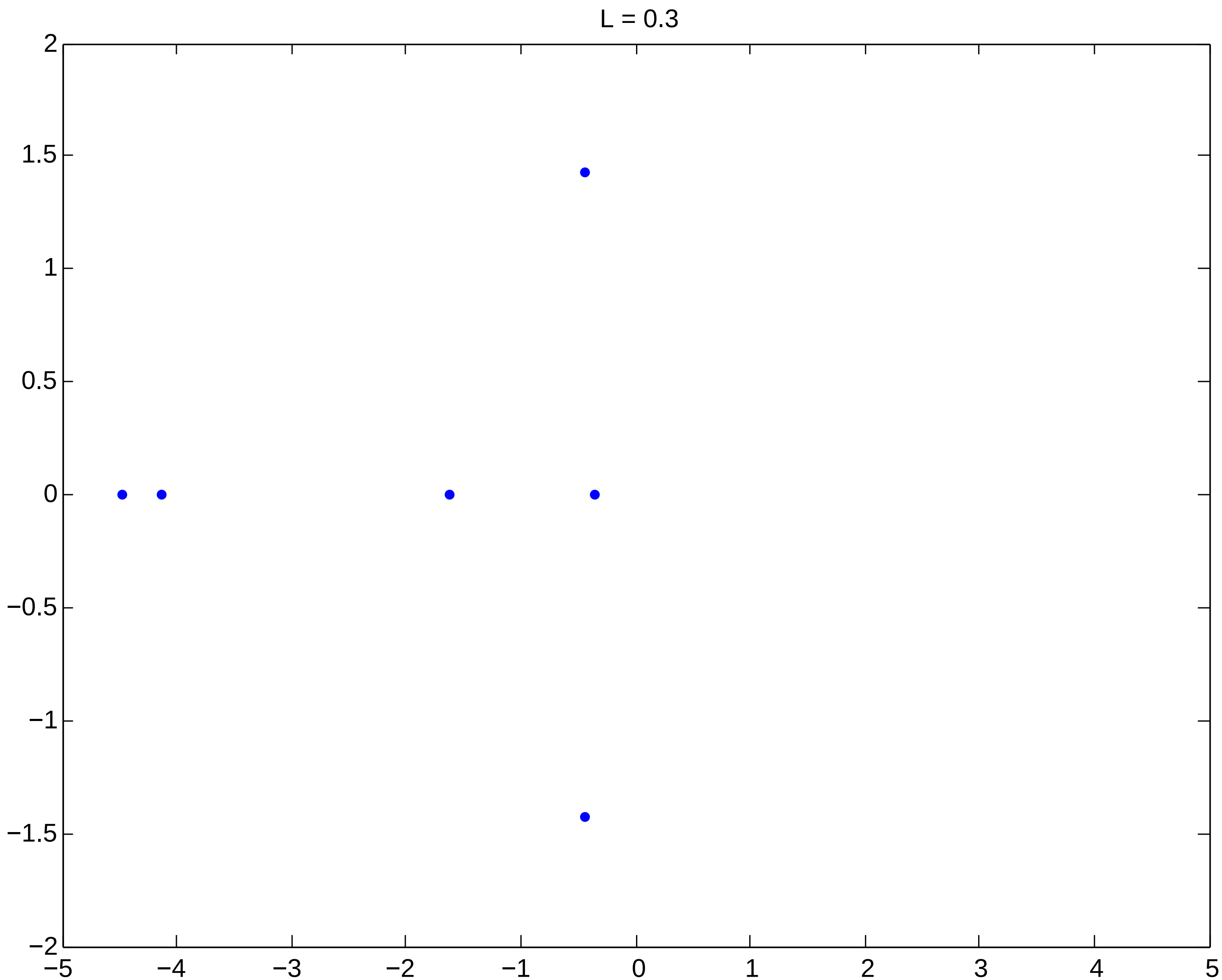
Stability analysis

Linearize about an equilibrium state:

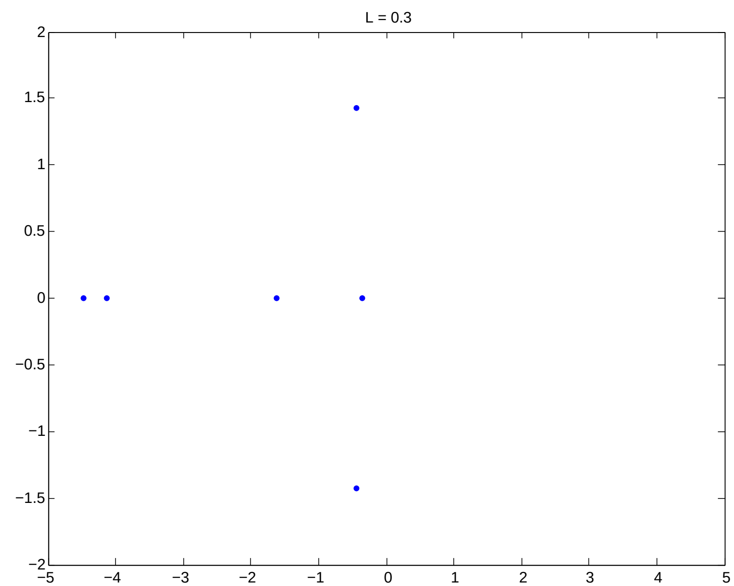
$$\frac{d}{dt}\begin{bmatrix}\delta u\\ \delta v\end{bmatrix} = \begin{bmatrix}\frac{D_u}{L^2}\frac{\partial^2}{\partial z^2} + f_u & f_v \\ g_u & \frac{D_u}{L^2}\frac{\partial^2}{\partial z^2} + g_v\end{bmatrix}\begin{bmatrix}\delta u\\ \delta v\end{bmatrix} = J\begin{bmatrix}\delta u\\ \delta v\end{bmatrix}$$

- 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 $\implies$ oscillations, a *Hopf bifurcation*

Bifurcation analysis



Subspace projections



- 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

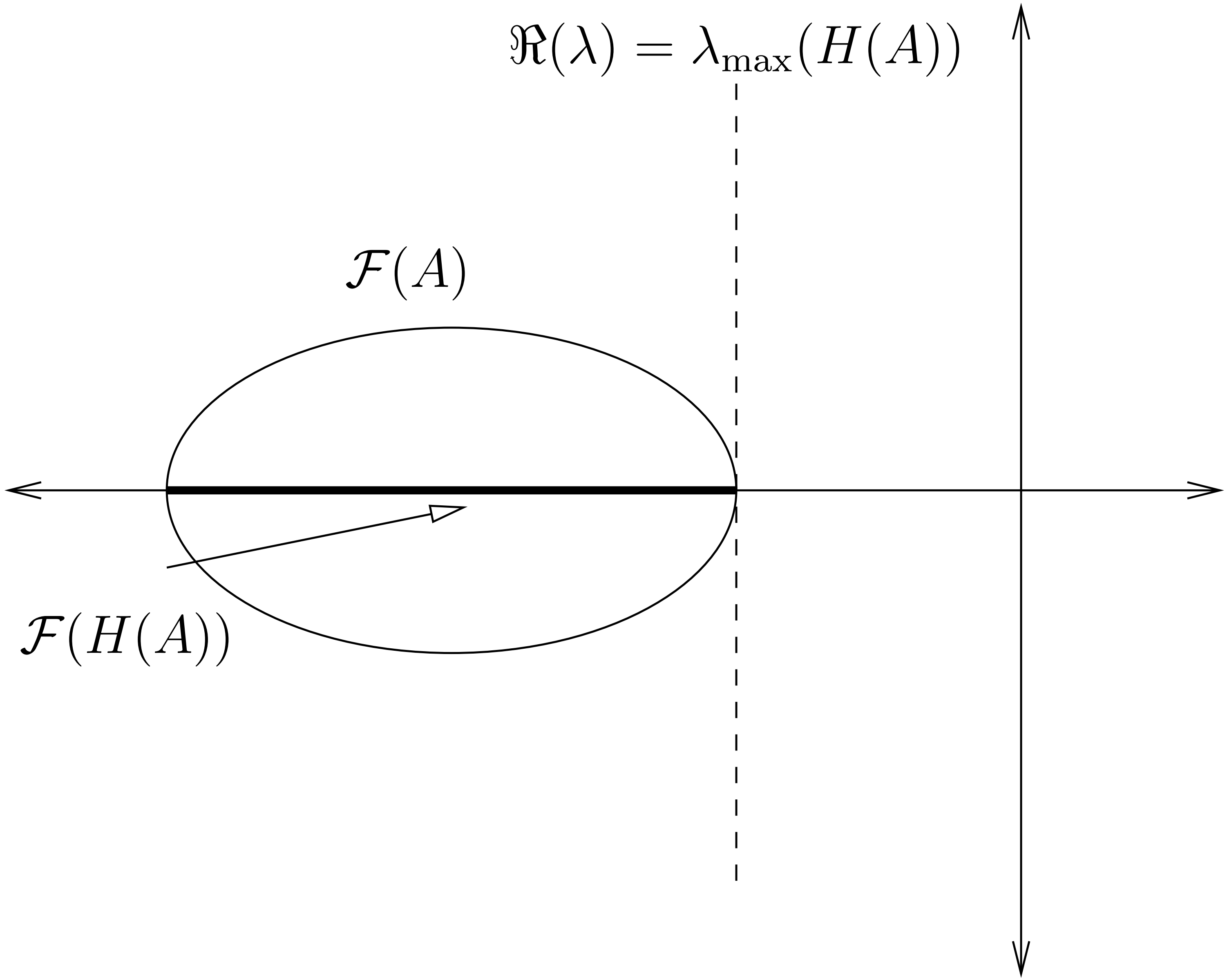
$$\mathcal{F}(A) := \{x^* A x : x^* x = 1\}$$

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

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

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

Bounding $\mathcal{F}(A)$

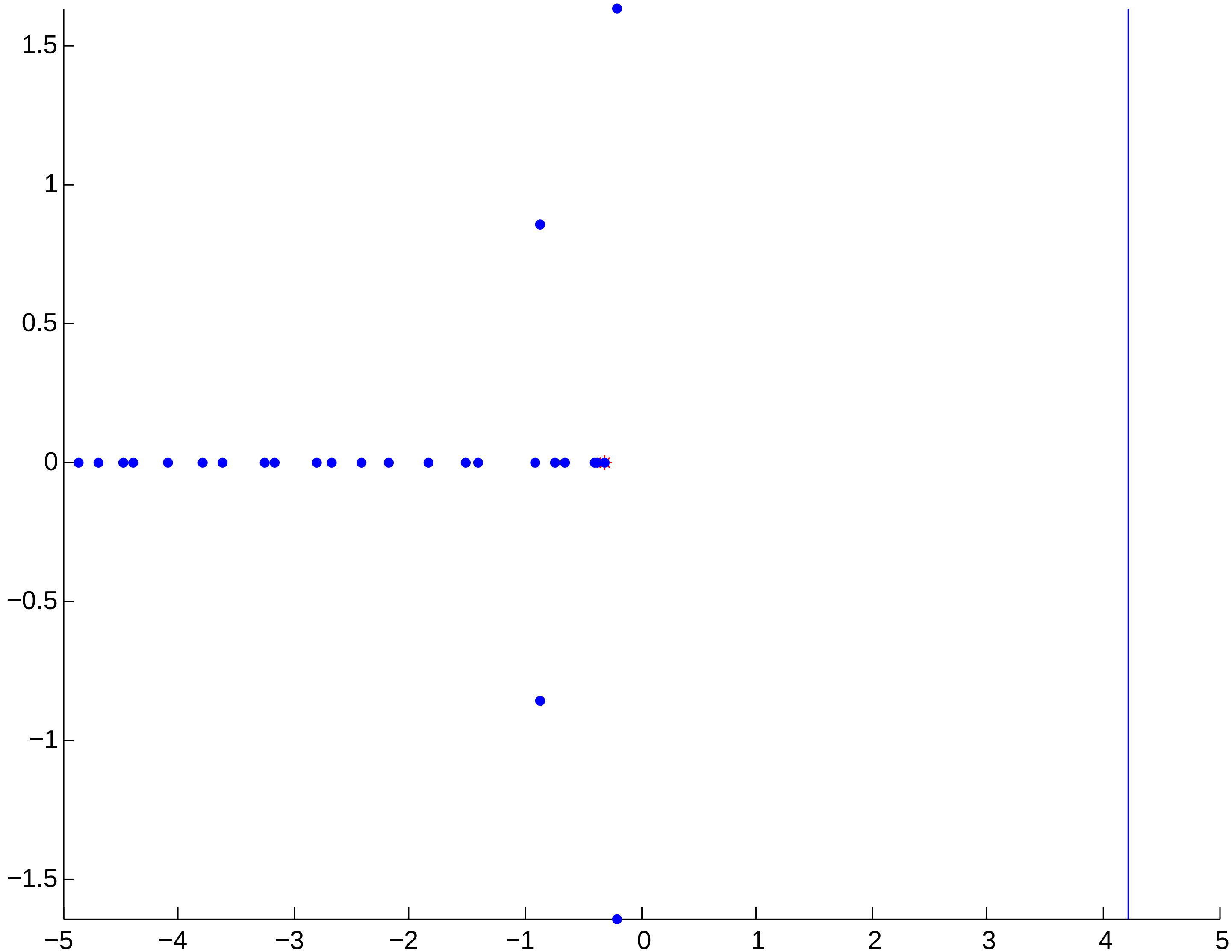


Field of values and bifurcation analysis

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

- 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 $y' = Jy$, 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.

Perturbations

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?

Pseudospectra

Might want to analyze *pseudospectra* instead of eigenvalues

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

- 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...

Block pseudospectral Gershgorin

Partition a matrix A into blocks:

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

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).

Arnoldi and Gershgorin

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

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.

Pseudo-spectral Bauer-Fike

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

A hybrid bound

For any $\gamma > 0$, define

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

Then

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

- 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
- $\hat{T}_{11} - \lambda I - \hat{T}_{12}(\hat{T}_{22} - \lambda I)^{-1} E_{21}$ 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)