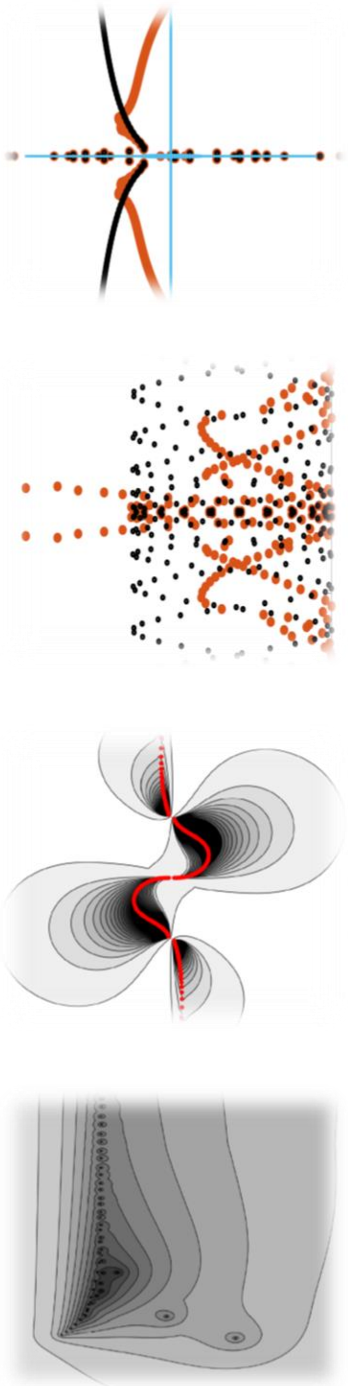

Discretization woes for NLEVPs

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24/05/2023

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Joint work with

Alex Townsend

(Cornell)

Nonlinear spectral problems (NEPs)

Many* NEPs are set in infinite-dimensional spaces.

Infinite-dimensional

Hilbert space

$$T(\lambda)\colon \mathcal{D}(T) \mapsto \mathcal{H}, \qquad \lambda \in \Omega \subset \mathbb{C}$$

$\lambda \longrightarrow T(\lambda)u$ holomorphic for all $u \in \mathcal{D}(T)$

$$\begin{aligned}
\mathrm{Sp}(T) &= \{\lambda \in \Omega\colon T(\lambda) \text{ is not invertible}\} \\
\mathrm{Sp}_{\mathrm{d}}(T) &= \{\lambda \in \mathrm{Sp}(T)\colon \lambda \text{ isolated}, T(\lambda) \text{ Fredholm}\} \\
\mathrm{Sp}_{\mathrm{ess}}(T) &= \mathrm{Sp}(T)\backslash \mathrm{Sp}_{\mathrm{d}}(T)
\end{aligned}$$

* 25/52 problems from NLEVP collection are discretized infinite-dimensional problems.

*A vast majority of applications of NEPs involve differential operators.

- Güttel, Tisseur, *"The nonlinear eigenvalue problem,"* **Acta Numerica**, 2017.
- Betcke, Higham, Mehrmann, Schröder, Tisseur, *"NLEVP: A collection of nonlinear eigenvalue problems,"* **ACM Trans. Math. Soft.**, 2013.

Discretization woes (examples later)

Often, we discretize to a matrix NEP

$$\lambda \longmapsto F(\lambda) \in \mathbb{C}^{n\times n}, \qquad \lambda \in \Omega \subset \mathbb{C}$$

But can cause serious issues:

- Spectral pollution (spurious eigenvalues).
- Spectral invisibility.
- Super-slow convergence (nonlinearity can make this even worse!)
- Ill-conditioning, even if $T(\lambda)$ is well-conditioned.
- Essential spectra, accumulating eigenvalues etc.
- Ghost essential spectra.

WARNING: Some inf-dim comp. spec. problems cannot be solved, regardless of computational power, time or model.

- C., "*The foundations of infinite-dimensional spectral computations,*" **PhD diss.**, University of Cambridge, 2020.

Computational tool #1: Pseudospectra

$$\mathcal{A}(\varepsilon) = \left\{E : \Omega \to \mathcal{B}(\mathcal{H}) \text{ holomorphic}: \sup_{\lambda\in\Omega} \|E(\lambda)\| < \varepsilon\right\}$$

$$\mathrm{Sp}_\varepsilon(T) = \bigcup_{E\in\mathcal{A}(\varepsilon)} \mathrm{Sp}(T+E) = \{\lambda \in \Omega : \|T(\lambda)^{-1}\|^{-1} < \varepsilon\}$$

Stability of spectrum

Characterization through resolvent

Computational tool #1: Pseudospectra

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FACT: $\|T(\lambda)^{-1}\|^{-1} = \min\left\{\sigma_{\inf}\big(T(\lambda)\big), \sigma_{\inf}(T(\lambda)^*)\right\}$

$$\sigma_{\inf}(A) = \inf\{\|Av\|\colon v \in \mathcal{D}(A), \|v\| = 1\}$$

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APPROXIMATION: $\gamma_n(\lambda) = \min\{\sigma_{\mathrm{inf}}(T(\lambda)\mathcal{P}_n^*), \sigma_{\mathrm{inf}}(T(\lambda)^*\mathcal{P}_n^*)\}$

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Rectangular sections

$\sigma_{\mathrm{inf}}\left(\mathcal{P}_{f(n)} T(\lambda) \mathcal{P}_n^*\right)$

Folding

$\sqrt{\sigma_{\mathrm{inf}}(\mathcal{P}_n T(\lambda)^* T(\lambda) \mathcal{P}_n^*)}$

- C., Hansen, *"The foundations of spectral computations via the solvability complexity index hierarchy,"* **J. Eur. Math. Soc.**, 2022.
- C., Townsend, *"Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems,"* **CPAM**, to appear.

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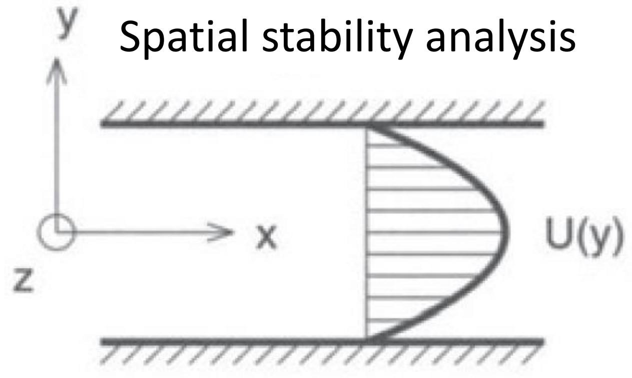
APPROXIMATION: $\gamma_n(\lambda) = \min\{\sigma_{\inf}(T(\lambda)\mathcal{P}_n^*), \sigma_{\inf}(T(\lambda)^*\mathcal{P}_n^*)\}$

THEOREM: Let $\Gamma_n(T, \varepsilon) = \{\lambda \in \Omega: \gamma_n(\lambda) < \varepsilon\}$, then (in the Attouch-Wets metric)

$$\lim_{n\to\infty} \Gamma_n(T, \varepsilon) = \mathrm{Sp}_\varepsilon(T), \qquad \Gamma_n(T, \varepsilon) \subset \mathrm{Sp}_\varepsilon(T).$$

$\sigma_{\inf}(A) = \inf\{\|Av\|: v \in \mathcal{D}(A), \|v\| = 1\}$

Example of verification: Orr-Sommerfeld



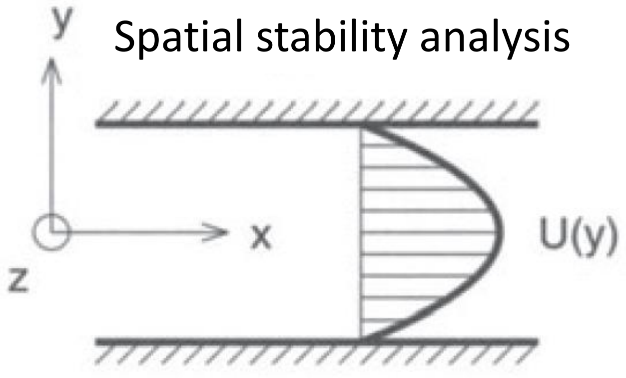
Poiseuille flow: $U(y) = 1 - y^2, y \in [-1,1]$

$R = 5772.22, \omega = 0.264002$

$A(\lambda)\phi = \left[\frac{1}{R}B(\lambda)^2 + i(\lambda U(y) - \omega)B(\lambda) + i\lambda U''(y)\right]\phi$

$B(\lambda)\phi = -\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2} + \lambda^2\phi,\ \langle\phi,\psi\rangle = \int_{-1}^{1}\phi\bar{\psi} + \frac{d\phi}{dy}\overline{\frac{d\psi}{dy}}\mathrm{d}y,\ T(\lambda) = B(\lambda)^{-1}A(\lambda)$

Example of verification: Orr-Sommerfeld



Poiseuille flow: $U(y) = 1 - y^2, y \in [-1,1]$

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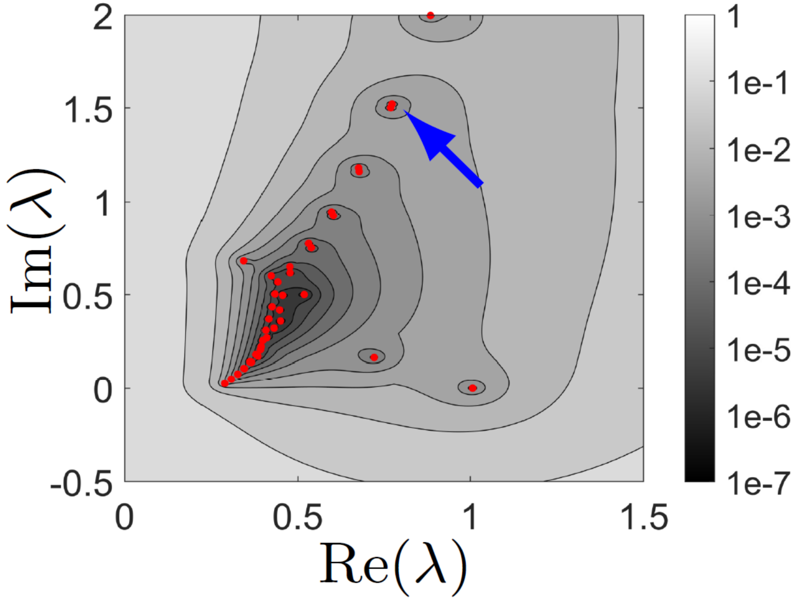
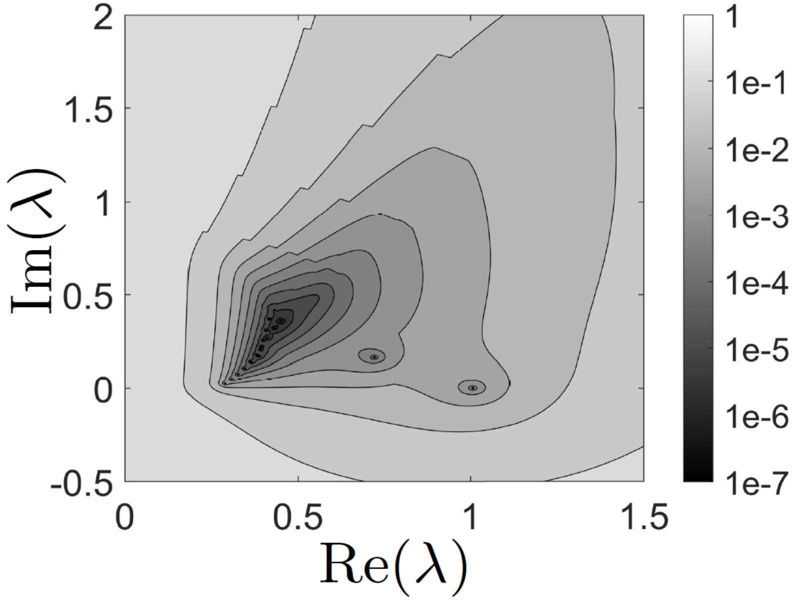
$T(\lambda) = B(\lambda)^{-1}A(\lambda)$

$\boxed{\{\lambda \in \Omega : \gamma_n(\lambda) < \varepsilon\} \subset \mathrm{Sp}_\varepsilon\ (T)}$

Cheb. Col., $n = 64$



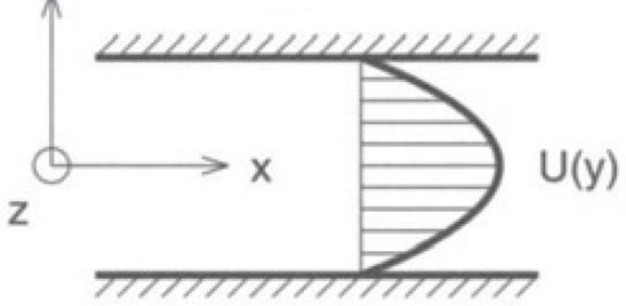
$\gamma_n, n = 64$



Which do we trust?

Example of verification: Orr-Sommerfeld

Spatial stability analysis



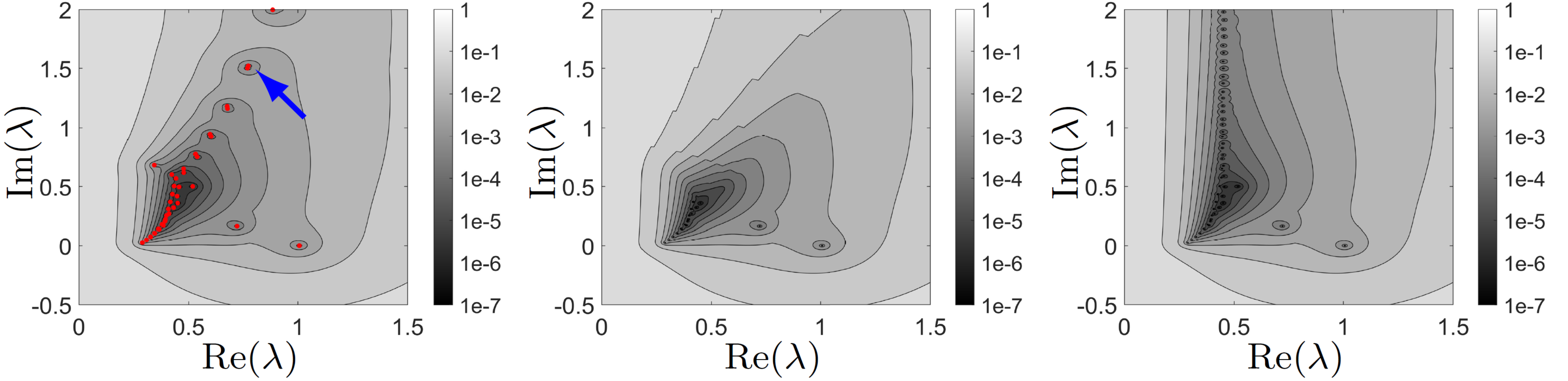
Poiseuille flow: $U(y) = 1 - y^2, y \in [-1,1]$

$R = 5772.22, \omega = 0.264002$

$T(\lambda) = B(\lambda)^{-1}A(\lambda)$

$\boxed{\{\lambda \in \Omega : \gamma_n(\lambda) < \varepsilon\} \subset \mathrm{Sp}_\varepsilon\,(T)}$

Cheb. Col., $n = 64$ | $\gamma_n, n = 64$ | Converged

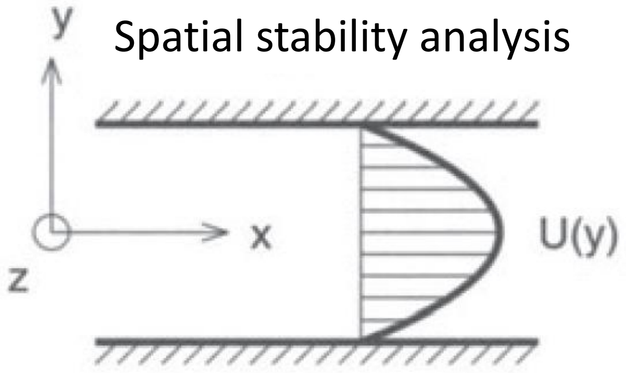


Example of verification: Orr-Sommerfeld

Poiseuille flow: $U(y) = 1 - y^2, y \in [-1,1]$

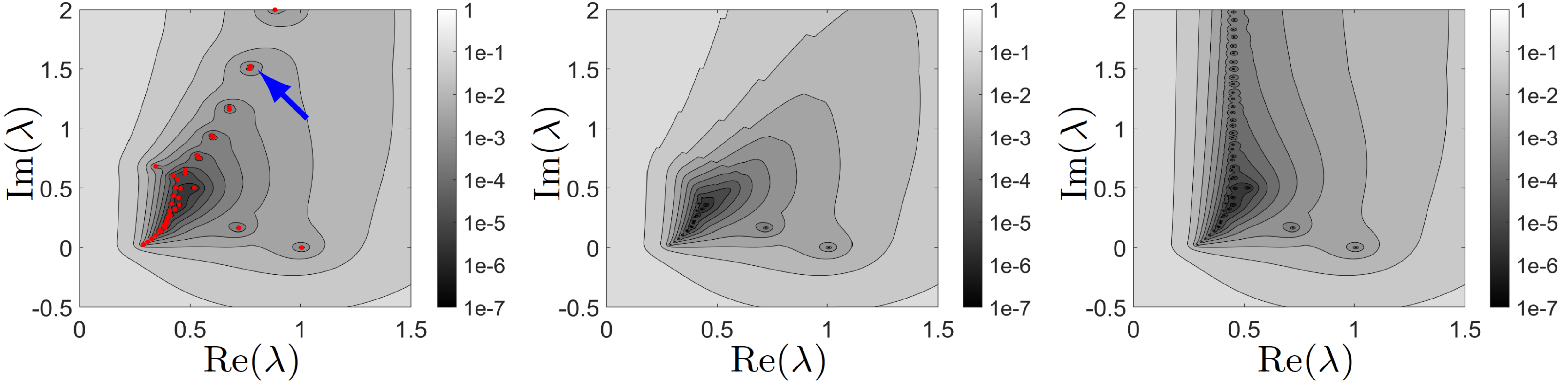
$R = 5772.22, \omega = 0.264002$

$T(\lambda) = B(\lambda)^{-1}A(\lambda)$



$\{\lambda \in \Omega: \gamma_n(\lambda) < \varepsilon\} \subset \mathrm{Sp}_\varepsilon\,(T)$

Cheb. Col., $n = 64$ | $\gamma_n, n = 64$ | Converged



NB: Standard method converges in this case but doesn't have verification.

Computational tool #2: Contour methods

KELDYSH's THEOREM: Suppose $\mathrm{Sp}_{\mathrm{ess}}(T) \cap \Omega = \emptyset$. Then for $z \in \Omega \backslash \mathrm{Sp}(T)$

$$T(z)^{-1} = V(z-J)^{-1}W^* + R(z)$$

- m is sum of all algebraic multiplicities of eigenvalues inside Ω.
- V & W are quasimatrices with m cols of right & left generalized eigenvectors.
- J consists of Jordan blocks.
- $R(z)$ is a bounded holomorphic remainder.

$\Longrightarrow$ use contour integration to convert to a linear pencil...

- Keldysh, *"On the characteristic values and characteristic functions of certain classes of non-self-adjoint equations,"* **Dokl. Akad. Nauk**, 1951.
- Keldysh, *"On the completeness of the eigenfunctions of some classes of non-self-adjoint linear operators,"* **UMN**, 1971.

InfBeyn algorithm

Let $\Gamma \subset \Omega$ be a contour enclosing m eigenvalues (and not touching $\mathrm{Sp}(T)$).

$$A_0 = \frac{1}{2\pi i}\int_\Gamma T(z)^{-1}\mathcal{V}\,\mathrm{d}z, \qquad A_1 = \frac{1}{2\pi i}\int_\Gamma zT(z)^{-1}\mathcal{V}\,\mathrm{d}z$$

Random vectors drawn form a Gaussian process

Computed with adaptive discretization sizes (e.g., ultraspherical spectral method)

Approximate through quadrature to obtain $\tilde{A}_0$ and $\tilde{A}_1$.

Eigenpairs (λ_j, x_j)
The eigenvectors of original problem are $\approx \mathcal{U}\Sigma_0 x_j$

Truncated SVD: $\tilde{A}_0 \approx \tilde{\mathcal{U}}\Sigma_0\tilde{V}_0^*$.

Form the linear pencil: $\tilde{F}(z) = \tilde{\mathcal{U}}^*\tilde{A}_1\tilde{V}_0 - z\tilde{\mathcal{U}}^*\tilde{A}_0\tilde{V}_0 \in \mathbb{C}^{m\times m}$.

NB: $m = \mathrm{Trace}\left(\frac{1}{2\pi i}\int_\Gamma T'(z)T(z)^{-1}\,\mathrm{d}z\right)$ can compute this (another story).

- Beyn, *"An integral method for solving nonlinear eigenvalue problems,"* **Linear Algebra Appl.**, 2012.
- C., Townsend, *"Avoiding discretization issues for nonlinear eigenvalue problem"*, preprint.

Stability and convergence result

Keldysh: $T(z)^{-1} = V(z-J)^{-1}W^* + R(z)$, let $M = \sup_{z\in\Omega}\|R(z)\|$.

Suppose that $\|\tilde{A}_j - A_j\| \leq \varepsilon$.

THEOREM: For sufficiently oversampled $\mathcal{V}$, with overwhelming probability,

$$\left|\sigma_{\inf}(F(z)) - \sigma_{\inf}(\tilde{F}(z))\right| \leq 2(\varepsilon + \|VJW^*\|\varepsilon/\sigma_m(VW^*) + |z|\varepsilon) \text{ (quad. err.)}$$

$$\mathrm{Sp}_{\frac{\varepsilon}{\|VW^*\|\|VW^*\mathcal{V}\|+M\varepsilon}}(T) \subset \mathrm{Sp}_\varepsilon(F) \subset \mathrm{Sp}_{\frac{\varepsilon}{\sigma_m(VW^*)\sigma_m(VW^*\mathcal{V})-M\varepsilon}}(T).$$

$\Longrightarrow$ **converges**
no spectral pollution
no spectral invisibility
method is stable

NOT a statement on computing $\mathrm{Sp}_\varepsilon(T)$
(the other algorithm does that!)

- C., Townsend, *"Avoiding discretization issues for nonlinear eigenvalue problem"*, preprint.
- Horning, Townsend, *"FEAST for differential eigenvalue problems,"* **SIAM J. Math. Anal.**, 2020.
- C., *"Computing semigroups with error control,"* **SIAM J. Math. Anal.**, 2022.

Stability bound

How to control quad error

Proof sketch

Keldysh: $T(z)^{-1} = V(z-J)^{-1}W^* + R(z)$, let $M = \sup_{z\in\Omega}\|R(z)\|$.
Introduce: $L_1 = (VW^*)^\dagger, \;\; L_2 = (VW^*\mathcal{V}V_0)^\dagger$.

$$T(z)^{-1}L_1F(z) = -VW^*\mathcal{V}V_0 + R(z)L_1F(z)$$
$$\sigma_{\inf}\big(F(z)\big) < \varepsilon \Longrightarrow \|T(z)^{-1}\| > \frac{\sigma_m(VW^*)\sigma_m(VW^*\mathcal{V})}{\varepsilon} - M$$

$$F(z)L_2[T(z)^{-1} - R(z)] = -VW^*$$
$$\|T(z)^{-1}\| > \varepsilon \Longrightarrow \sigma_{\inf}\big(F(z)\big) < \frac{\|VW^*\|\|VW^*\mathcal{V}\|}{1-M\varepsilon}\varepsilon$$

Use results from inf dim randomized NLA to bound terms with a $\mathcal{V}$.

- C., Townsend, *"Avoiding discretization issues for nonlinear eigenvalue problem"*, preprint.

Example 1: One-dimensional acoustic wave

acoustic_wave_1d from NLEVP collection.

$$\frac{\mathrm{d}^2 p}{\mathrm{d}x^2} + 4\pi^2\lambda^2 p = 0, \qquad p(0) = 0, \qquad \chi p'(1) + 2\pi i\lambda p(1) = 0$$

p corresponds to acoustic pressure.

Resonant frequencies: $\lambda_k = \dfrac{\tan^{-1}(i\chi)}{2\pi} + \dfrac{k}{2}, \quad k \in \mathbb{Z}$

Discretized using FEM ($n =$ discretization size)

Example 1: One-dimensional acoustic wave

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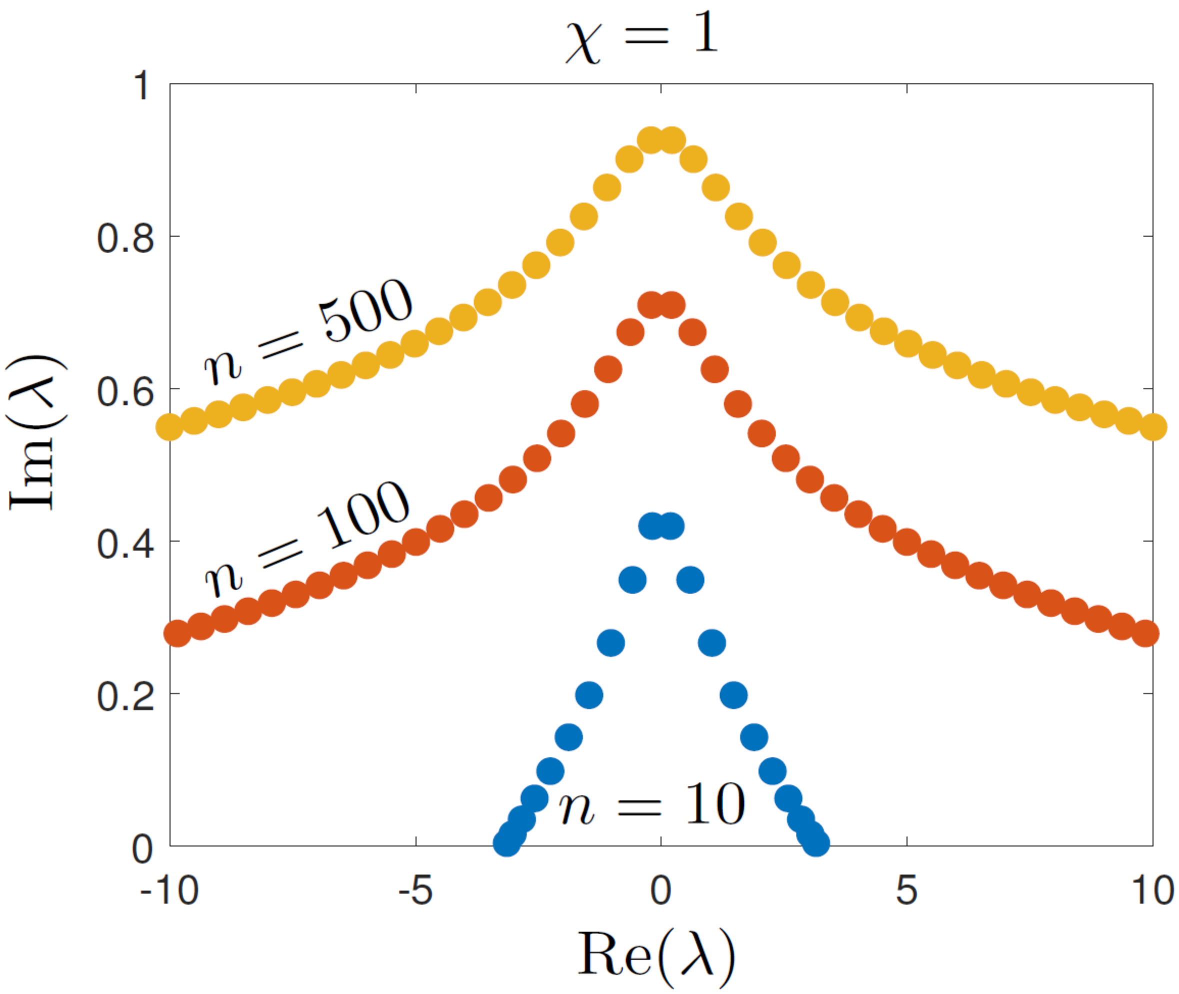

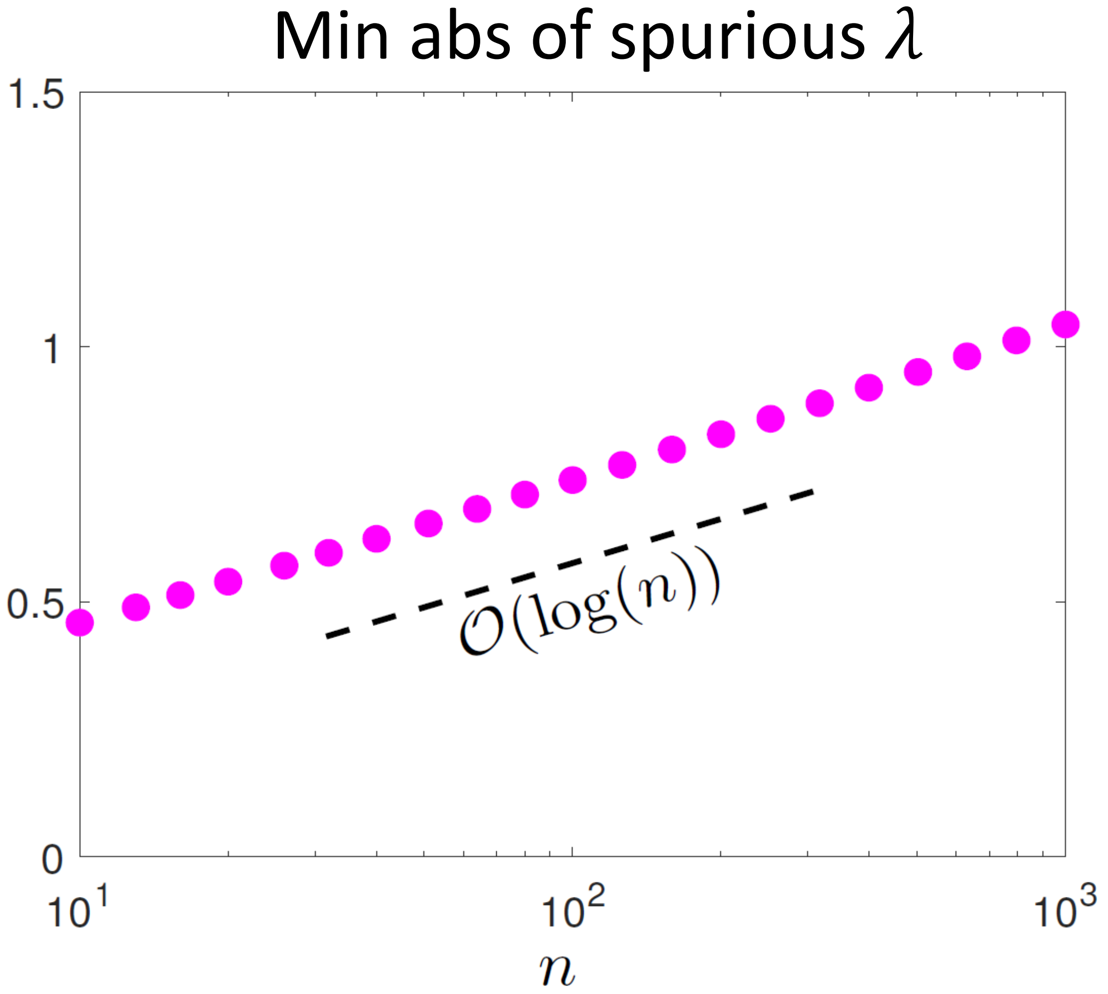

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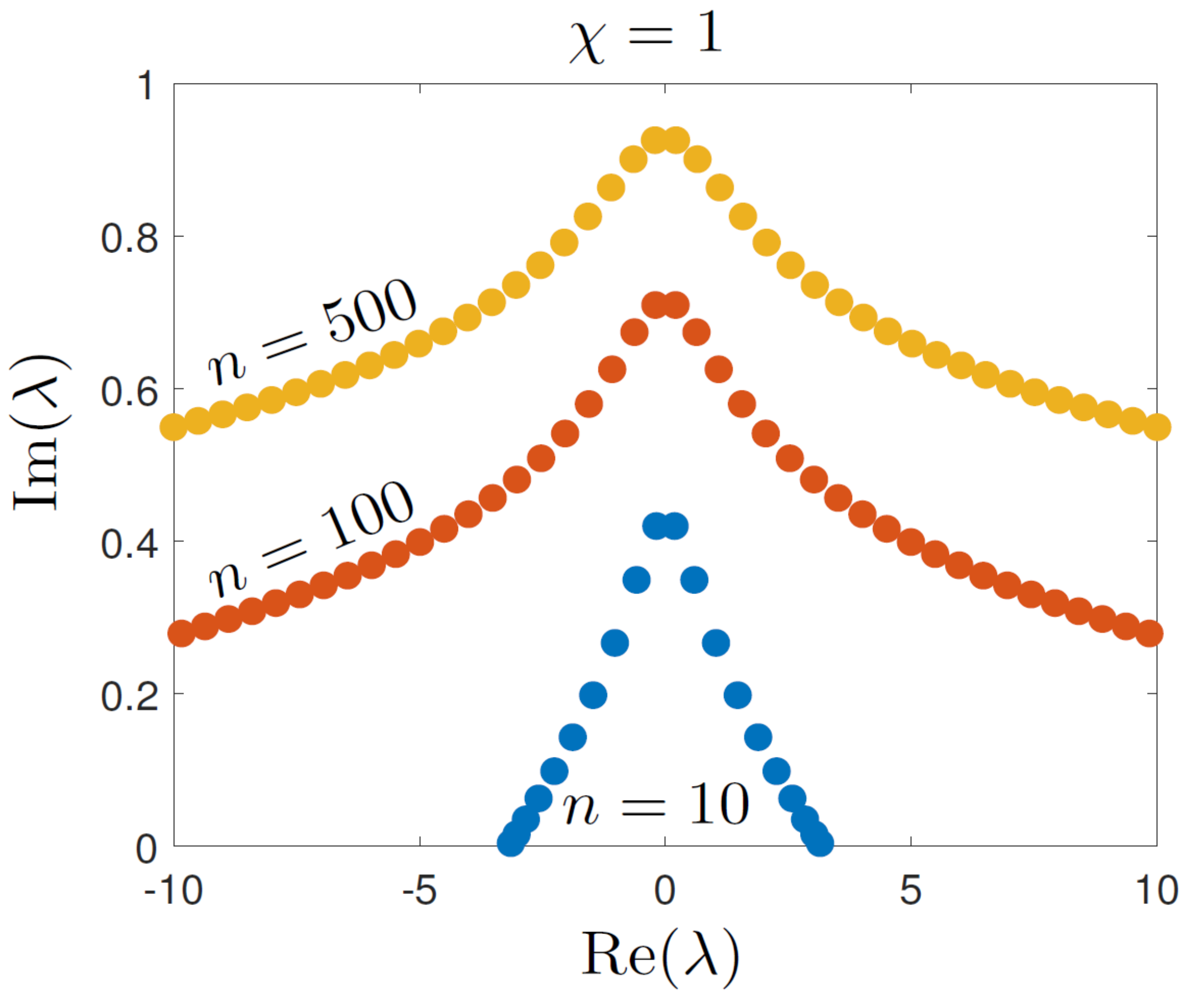
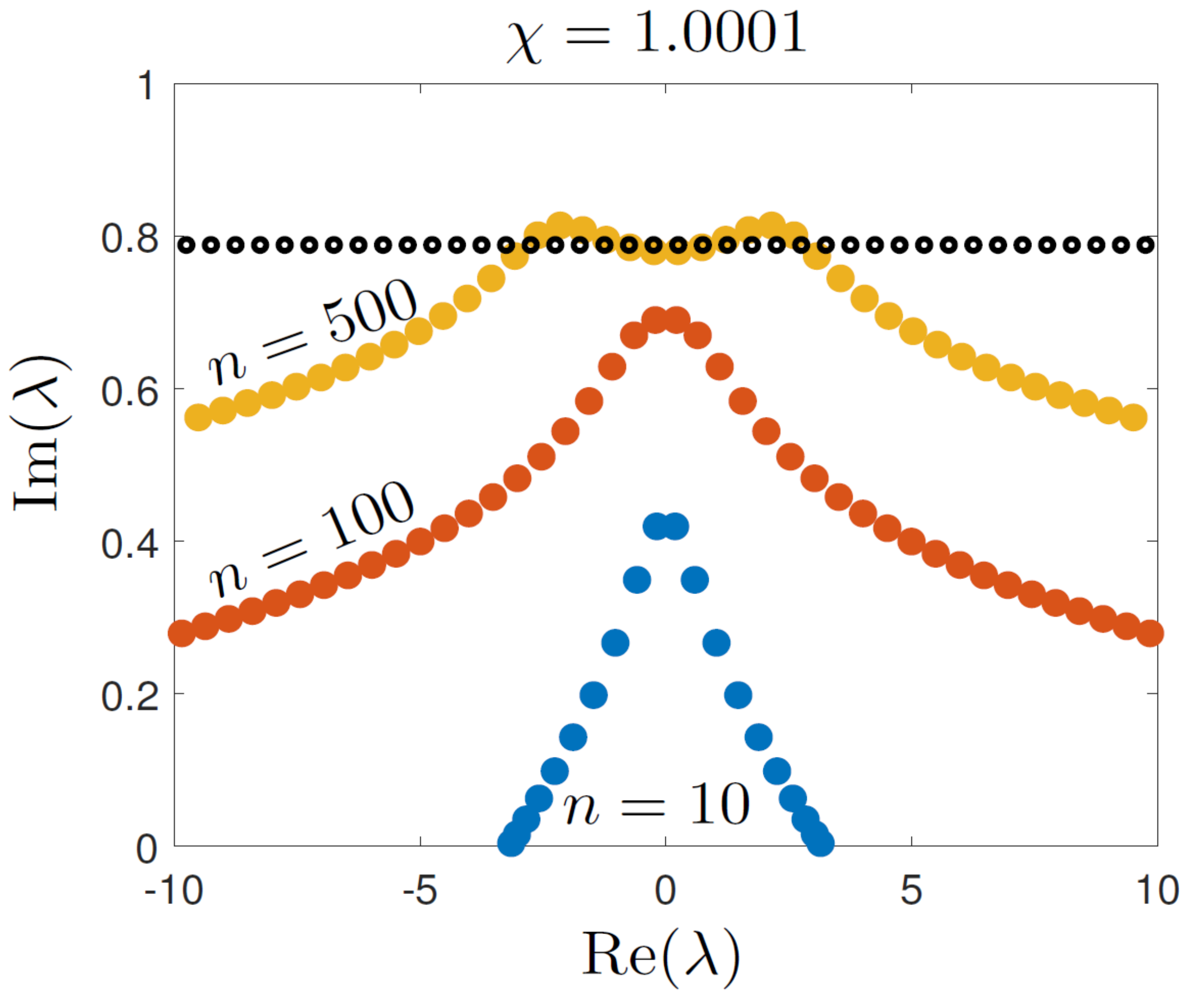
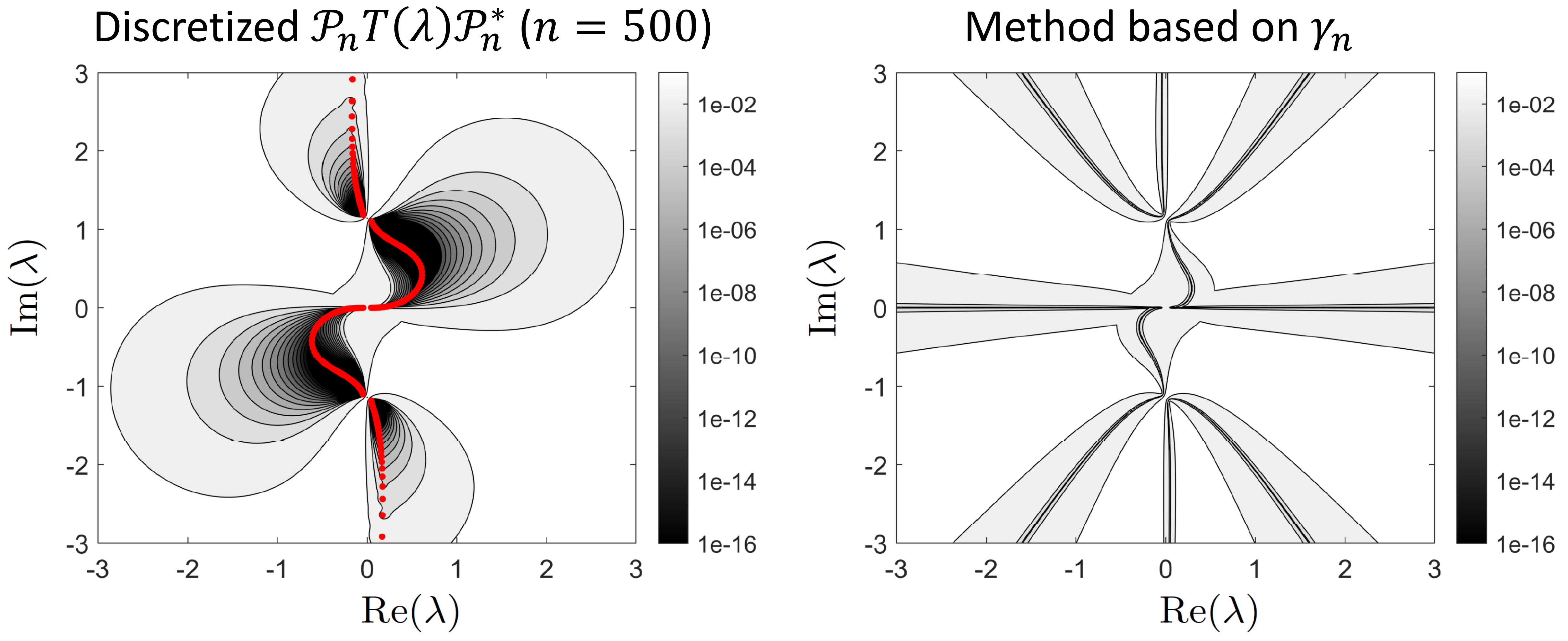




butterfly from NLEVP collection
$T(\lambda) = F(\lambda, S)$
S bilateral shift on $l^2(\mathbb{Z})$
F a rational function

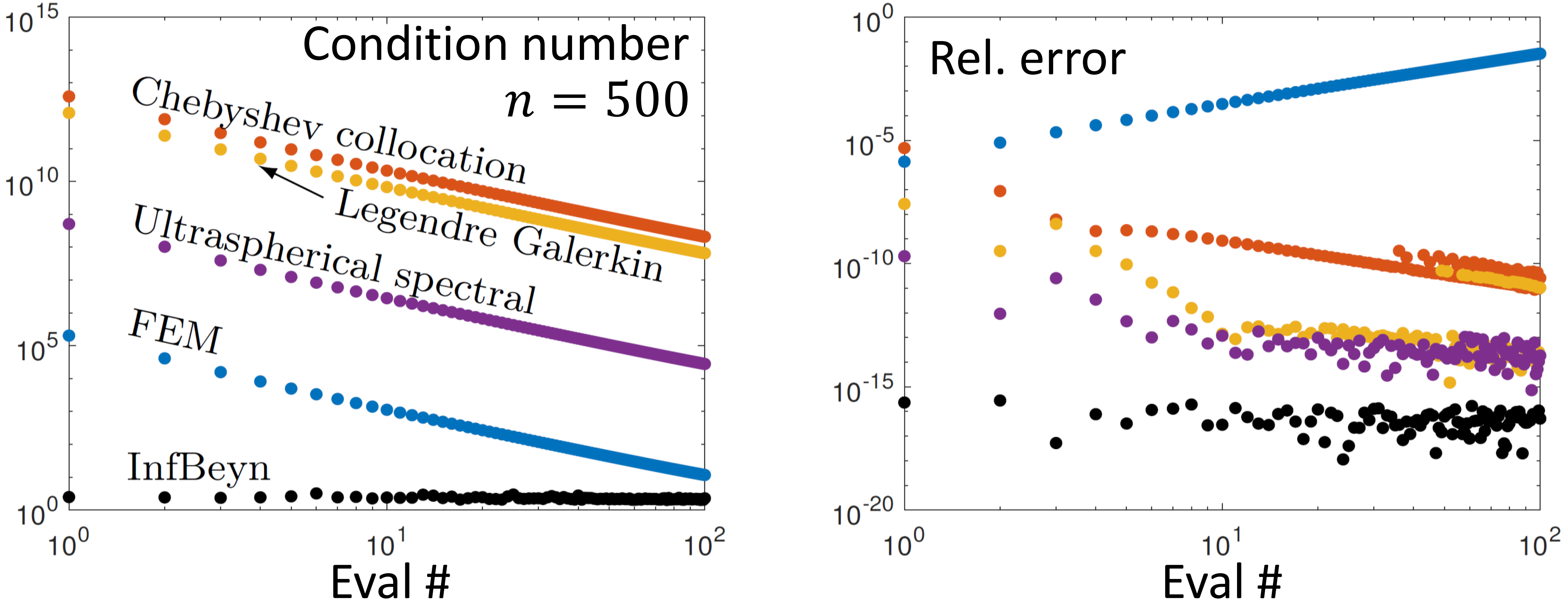
Example 2: Butterfly



Example 3: Loaded string

damped_beam from NLEVP collection.

$$-\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} = \lambda u, \qquad u(0) = 0, \qquad u'(1) + \frac{\lambda}{\lambda - 1} u(1) = 0.$$



Example 4: Planar waveguide

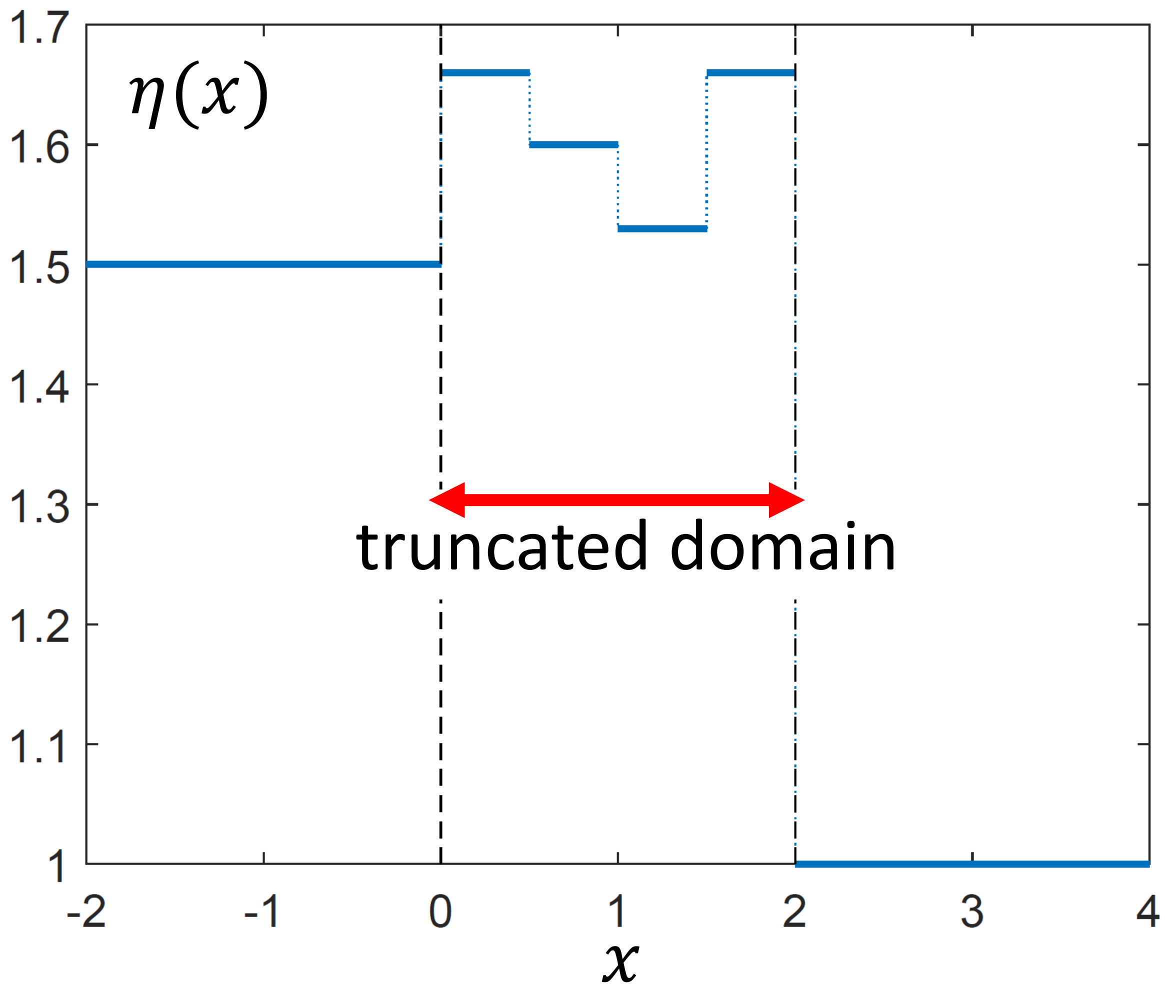
planar_waveguide from NLEVP collection.

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} + k^2\big(\eta^2 - \mu(\lambda)\big)\phi = 0$$

$$\mu(\lambda) = \frac{\delta_+}{k^2} + \frac{\delta_-}{8k^2\lambda^2} + \frac{\lambda^2}{k^2}$$

$$\frac{\mathrm{d}\phi}{\mathrm{d}x}(0) + \left(\frac{\delta_-}{2\lambda} - \lambda\right)\phi(0) = 0$$

$$\frac{\mathrm{d}\phi}{\mathrm{d}x}(2) + \left(\frac{\delta_-}{2\lambda} + \lambda\right)\phi(2) = 0$$

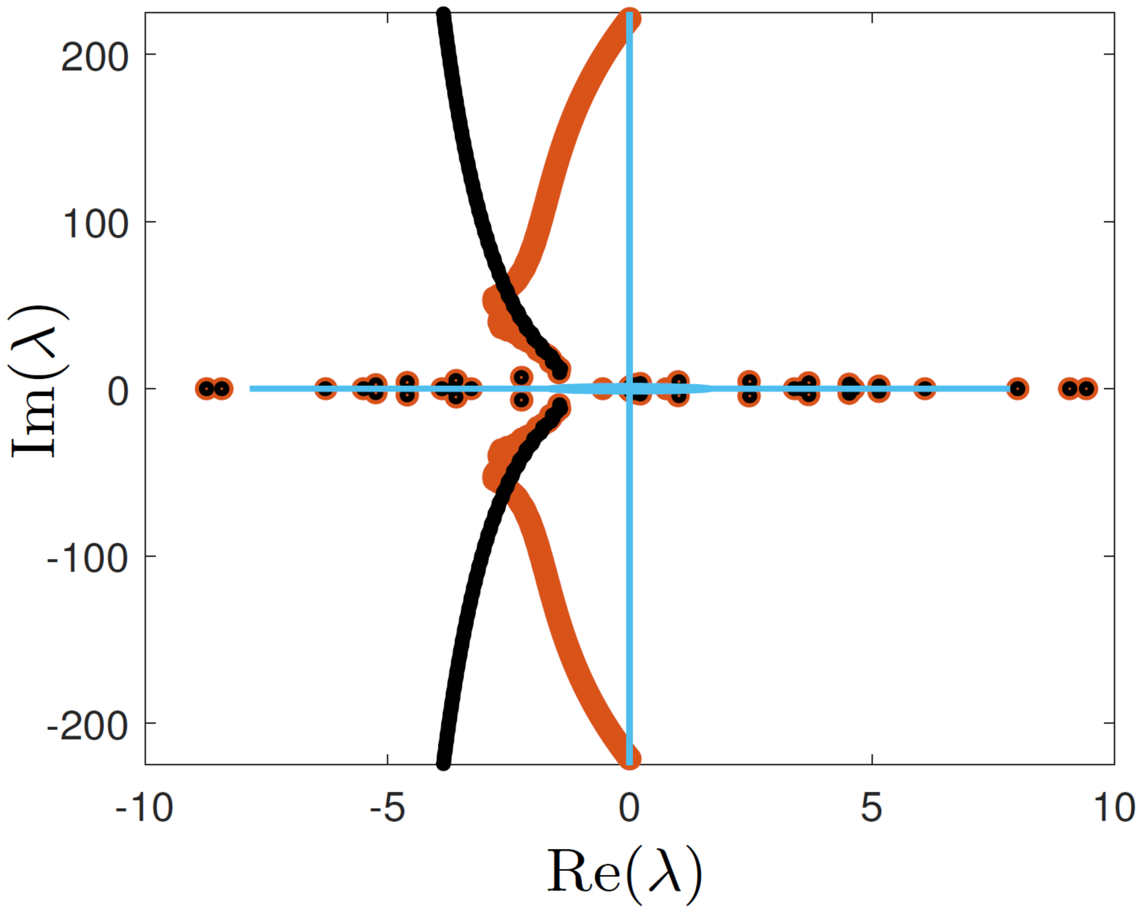


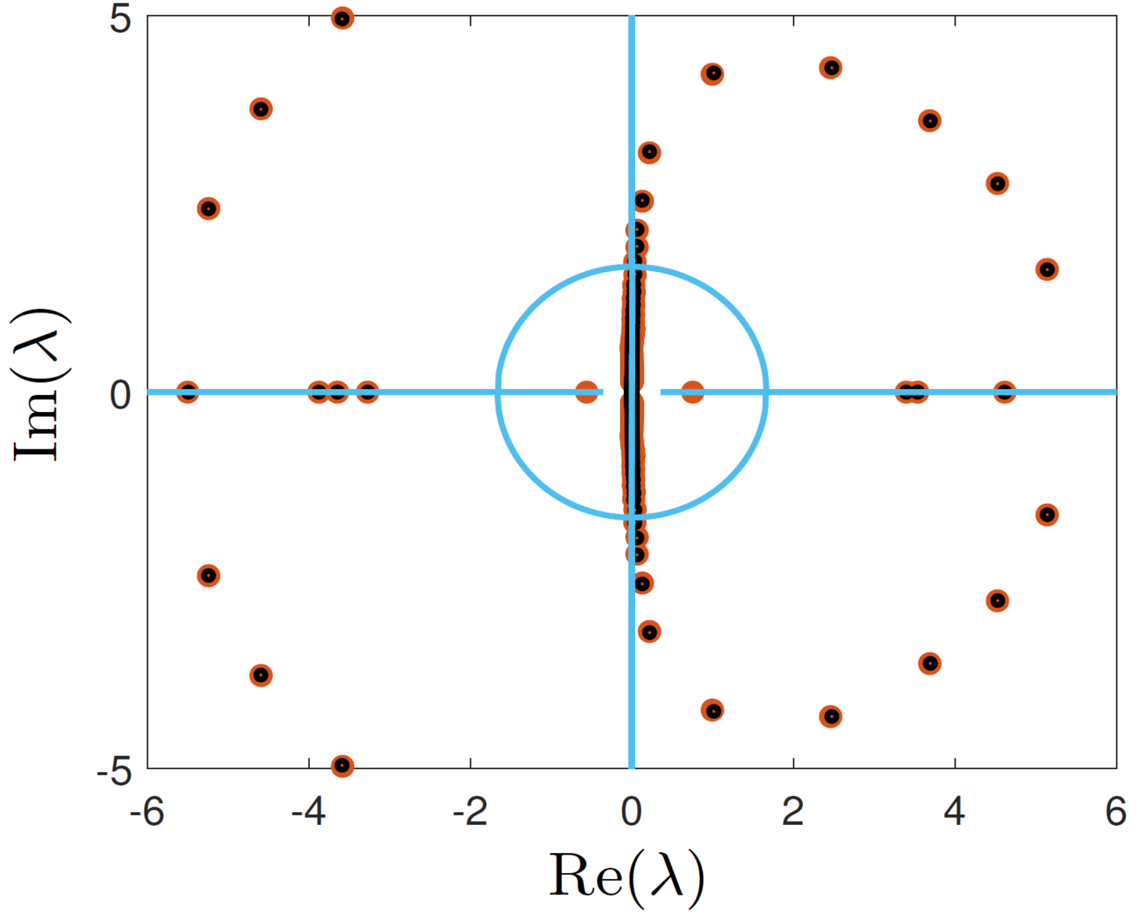
η corresponds to refractive index.

λ correspond to guided and leaky modes.

Discretized using FEM ($n = 129$, default)

Example 4: Planar waveguide





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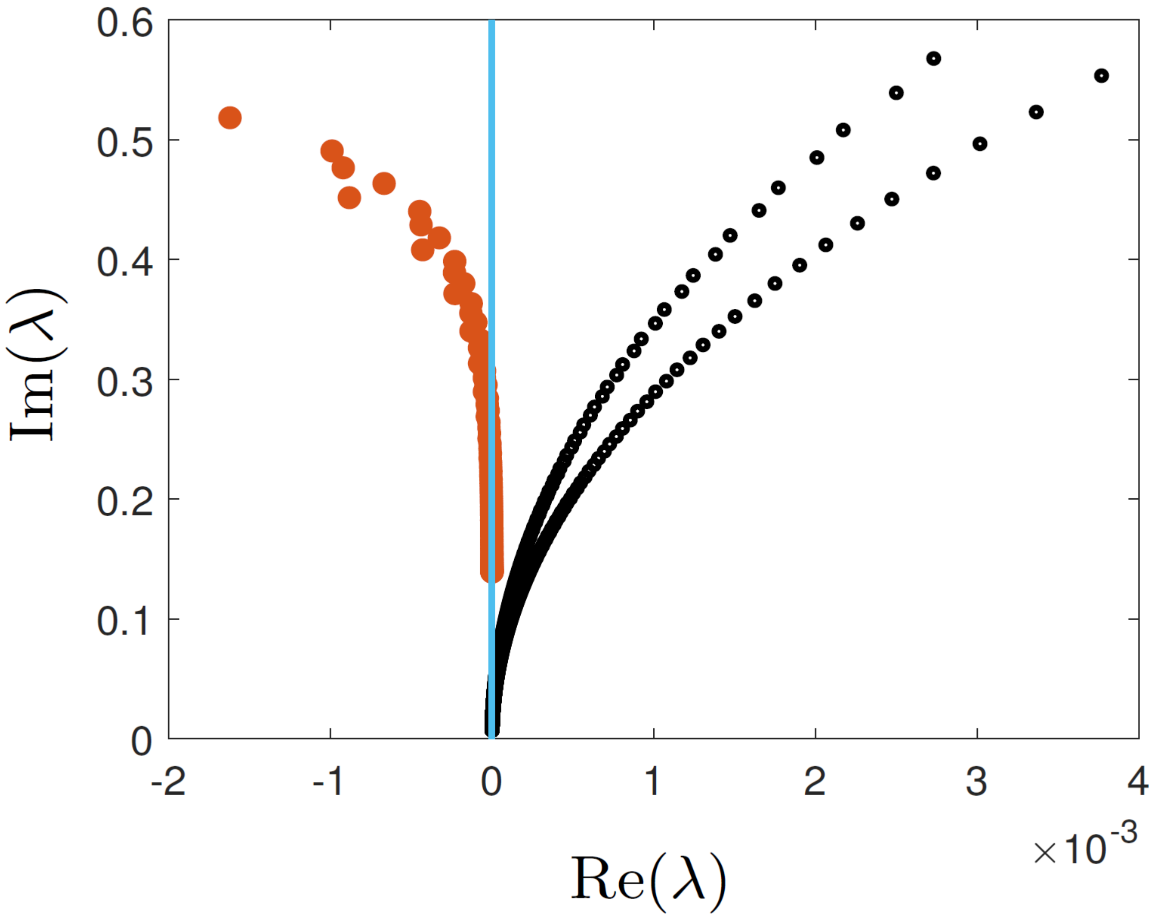
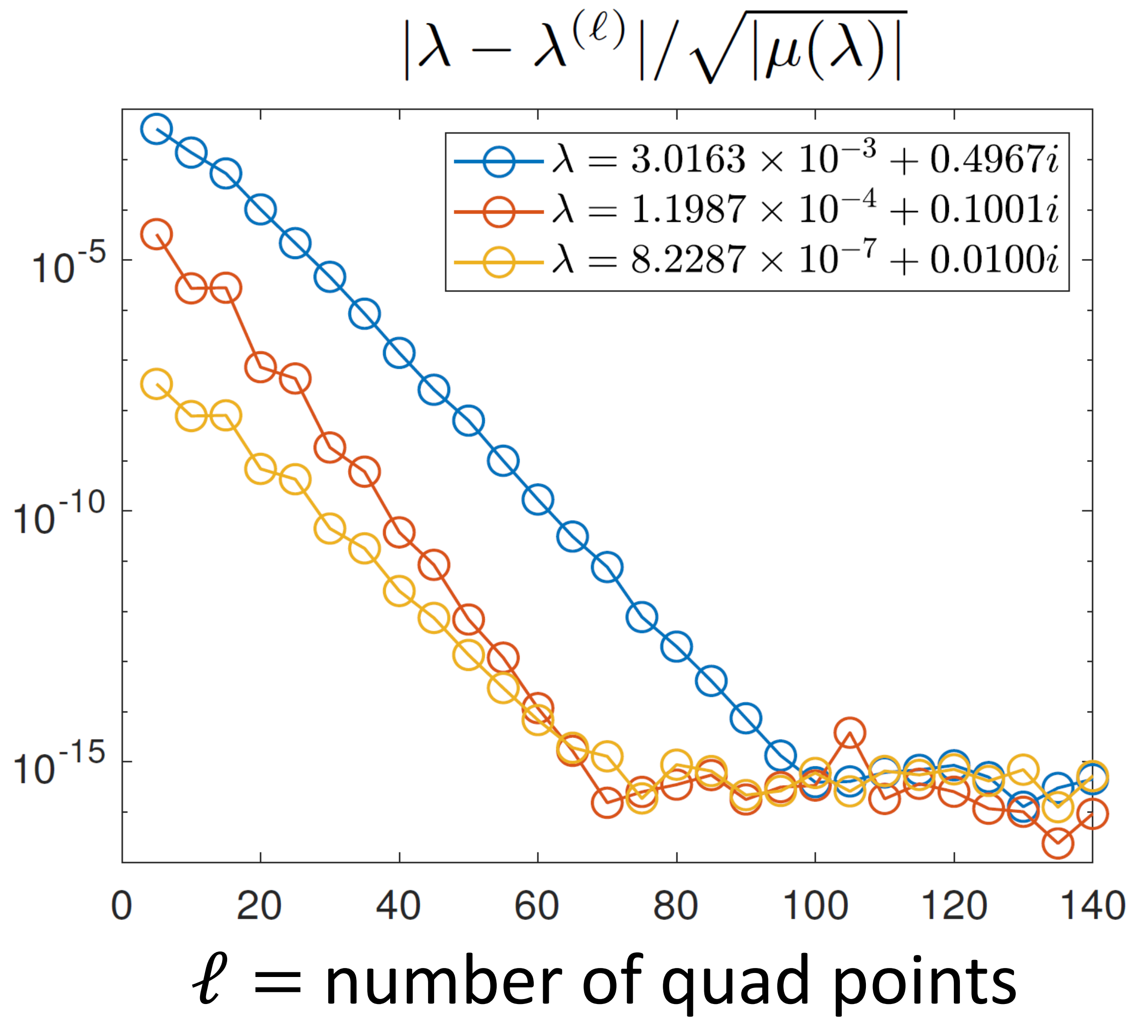
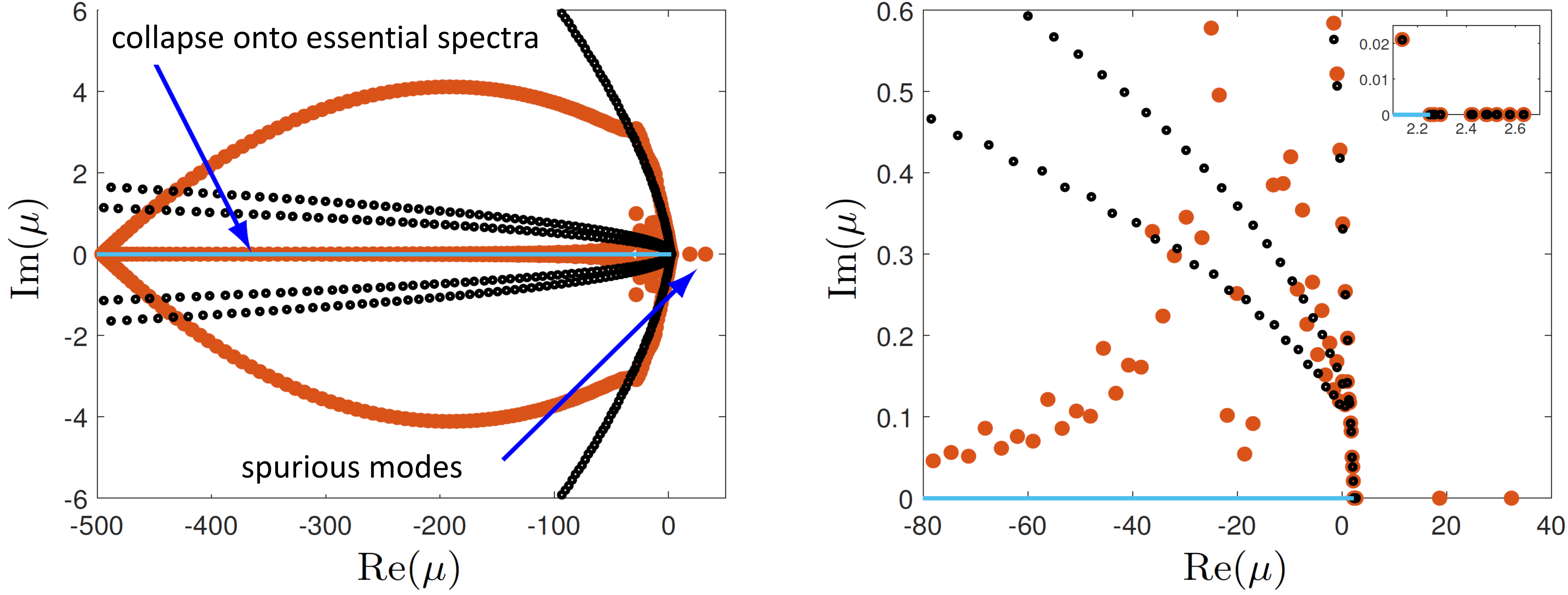




Example 4: Planar waveguide



Bigger picture

- **Foundations:** Classify difficulty of computational problems.
  - Prove that algorithms are optimal (in any given computational model).
  - Find assumptions and methods for computational goals.
- A new suite of "infinite-dimensional" algorithms. **Solve-then-discretize**.
  - **Methods built on $\boldsymbol{\sigma_{\mathrm{inf}}(T)}$**, e.g., compute $\sigma_{\mathrm{inf}}(T\mathcal{P}_n^*)$ or $\sqrt{\sigma_{\mathrm{inf}}(\mathcal{P}_n T^* T \mathcal{P}_n^*)}$
    - Spectra with error control (including essential spectrum).
    - Pseudospectra, stability bounds etc.
    - More exotic features such as fractal dimensions.
  - **Methods built on <u>adaptively</u> computing $\boldsymbol{(A - zI)^{-1}}$ or $\boldsymbol{T(z)^{-1}}$**
    - Contour methods: discrete spectra for linear and nonlinear pencils.
    - Convolution methods: spectral measures of self-adjoint and unitary operators.
    - Functions of operators with error control.

Summary for NEPs

- Discretization can cause serious issues.

Example	Observed discretization woes
`acoustic_wave_1d`	spurious eigenvalues slow convergence
`acoustic_wave_2d`	spurious eigenvalues wrong multiplicity
`butterfly`	spectral pollution missed spectra wrong pseudospectra
`damped_beam`	slow convergence resolved eigenfunctions with inaccurate eigenvalues
`loaded_string`	ill-conditioning from discretization
`planar_waveguide`	collapse onto ghost essential spectrum failure for accumulating eigenvalues spectral pollution

- **InfBeyn** overcomes these in regions of discrete spectra: **convergent, stable, efficient**.
- Compute pseudospectra (of generic pencils) with explicit **error control**

More on this program: **www.damtp.cam.ac.uk/user/mjc249/home.html**

Code: **https://github.com/MColbrook/infNEP**

- C., Townsend, *"Avoiding discretization issues for nonlinear eigenvalue problem"*, preprint.

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