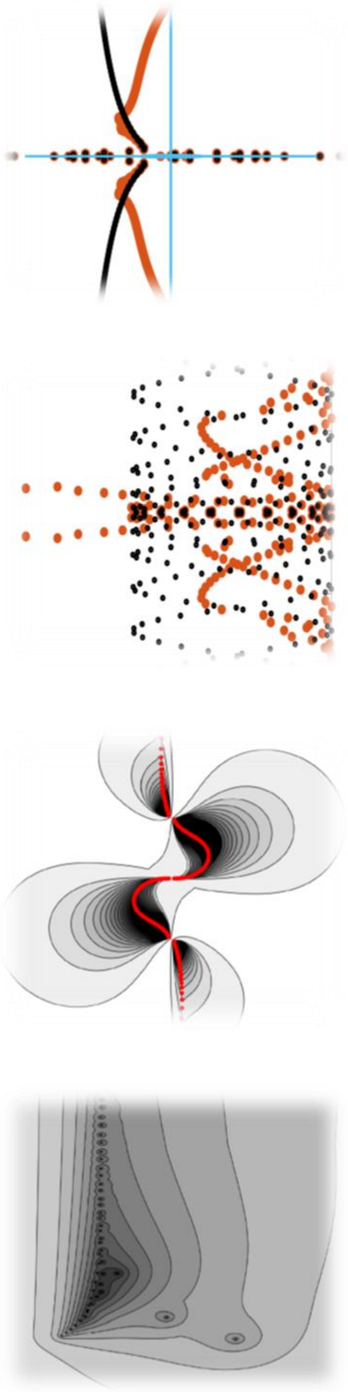


Taming Discretization Challenges for Nonlinear Eigenvalue Problems!

Matthew Colbrook
University of Cambridge
26/07/2023

Joint work with
Alex Townsend
(Cornell)

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

What is a nonlinear eigenvalue problem?

2 S. GÜTTEL AND F. TISSEUR

1. Introduction

Nonlinear eigenvalue problems arise in many areas of computational science and engineering, including acoustics, control theory, fluid mechanics and structural engineering. The fundamental formulation of such problems is given in the following definition.

Definition 1.1. Given a non-empty open set $\Omega \subseteq \mathbb{C}$ and a matrix-valued function $F : \Omega \to \mathbb{C}^{n \times n}$, the *nonlinear eigenvalue problem* (NEP) consists of finding scalars $\lambda \in \Omega$ (the *eigenvalues*) and nonzero vectors $v \in \mathbb{C}^n$ and $w \in \mathbb{C}^n$ (right and left *eigenvectors*) such that

$$F(\lambda)v = 0, \quad w^* F(\lambda) = 0^*.$$

Stefan Güttel

Françoise Tisseur

- Güttel, Tisseur, *"The nonlinear eigenvalue problem,"* **Acta Numerica**, 2017.

Nonlinear ~~eigenvalue~~ *spectral* problems (NEPs)

Many* NEPs are set in infinite-dimensional spaces.

Infinite-dimensional **Hilbert space**

For every $\lambda \in \Omega \subset \mathbb{C}$, $\quad T(\lambda): \mathcal{D}(T) \mapsto \mathcal{H}$

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

$T(\lambda)$ **linear** for fixed λ

Spectral sets

$$\mathrm{Sp}(T) = \{\lambda \in \Omega : T(\lambda) \text{ is not invertible}\}$$

$$\mathrm{Sp}_{\mathrm{d}}(T) = \{\lambda \in \mathrm{Sp}(T) : \lambda \text{ isolated}, T(\lambda) \text{ Fredholm}\}$$

$$\mathrm{Sp}_{\mathrm{ess}}(T) = \mathrm{Sp}(T) \backslash \mathrm{Sp}_{\mathrm{d}}(T)$$

Fun fact: $\mathrm{Sp}_{\mathrm{ess}}(T)$ can exist in finite dimensions! This doesn't happen in the linear case.

* Most applications of NEPs involve differential operators.

NLEVP collection: a standard benchmark

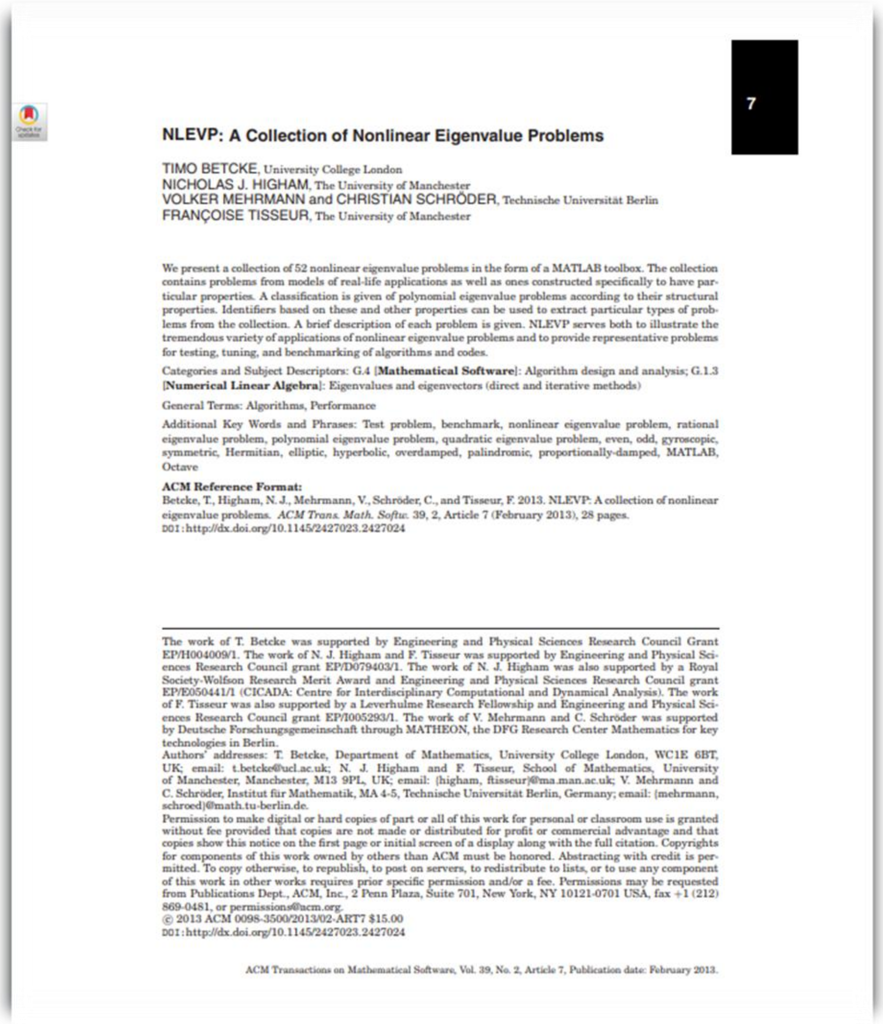
Timo Betcke

Nicholas Higham

Françoise Tisseur

Volker Mehrmann

Christian Schröder



7

NLEVP: A Collection of Nonlinear Eigenvalue Problems

TIMO BETCKE, University College London
NICHOLAS J. HIGHAM, The University of Manchester
VOLKER MEHRMANN and CHRISTIAN SCHRÖDER, Technische Universität Berlin
FRANÇOISE TISSEUR, The University of Manchester

We present a collection of 52 nonlinear eigenvalue problems in the form of a MATLAB toolbox. The collection contains problems from models of real-life applications as well as ones constructed specifically to have particular properties. A classification is given of polynomial eigenvalue problems according to their structural properties. Identifiers based on these and other properties can be used to extract particular types of problems from the collection. A brief description of each problem is given. NLEVP serves both to illustrate the tremendous variety of applications of nonlinear eigenvalue problems and to provide representative problems for testing, tuning, and benchmarking of algorithms and codes.

Categories and Subject Descriptors: G.4 [**Mathematical Software**]: Algorithm design and analysis; G.1.3 [**Numerical Linear Algebra**]: Eigenvalues and eigenvectors (direct and iterative methods)

General Terms: Algorithms, Performance

Additional Key Words and Phrases: Test problem, benchmark, nonlinear eigenvalue problem, rational eigenvalue problem, polynomial eigenvalue problem, quadratic eigenvalue problem, even, odd, gyroscopic, symmetric, Hermitian, elliptic, hyperbolic, overdamped, palindromic, proportionally-damped, MATLAB, Octave

ACM Reference Format:
Betcke, T., Higham, N. J., Mehrmann, V., Schröder, C., and Tisseur, F. 2013. NLEVP: A collection of nonlinear eigenvalue problems. *ACM Trans. Math. Softw.* 39, 2, Article 7 (February 2013), 28 pages.
DOI:http://dx.doi.org/10.1145/2427023.2427024

The work of T. Betcke was supported by Engineering and Physical Sciences Research Council Grant EP/H004009/1. The work of N. J. Higham and F. Tisseur was supported by Engineering and Physical Sciences Research Council grant EP/D079403/1. The work of N. J. Higham was also supported by a Royal Society-Wolfson Research Merit Award and Engineering and Physical Sciences Research Council grant EP/E050441/1 (CICADA: Centre for Interdisciplinary Computational and Dynamical Analysis). The work of F. Tisseur was also supported by a Leverhulme Research Fellowship and Engineering and Physical Sciences Research Council grant EP/I005293/1. The work of V. Mehrmann and C. Schröder was supported by Deutsche Forschungsgemeinschaft through MATHEON, the DFG Research Center Mathematics for key technologies in Berlin.

Authors' addresses: T. Betcke, Department of Mathematics, University College London, WC1E 6BT, UK; email: t.betcke@ucl.ac.uk; N. J. Higham and F. Tisseur, School of Mathematics, University of Manchester, Manchester, M13 9PL, UK; email: {higham, ftisseur}@ma.man.ac.uk; V. Mehrmann and C. Schröder, Institut für Mathematik, MA 4-5, Technische Universität Berlin, Germany; email: {mehrmann, schroed}@math.tu-berlin.de.

DOI:http://dx.doi.org/10.1145/2427023.2427024

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

- Betcke, Higham, Mehrmann, Schröder, Tisseur, *"NLEVP: A collection of nonlinear eigenvalue problems,"* **ACM Trans. Math. Soft.**, 2013.

Example: 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.

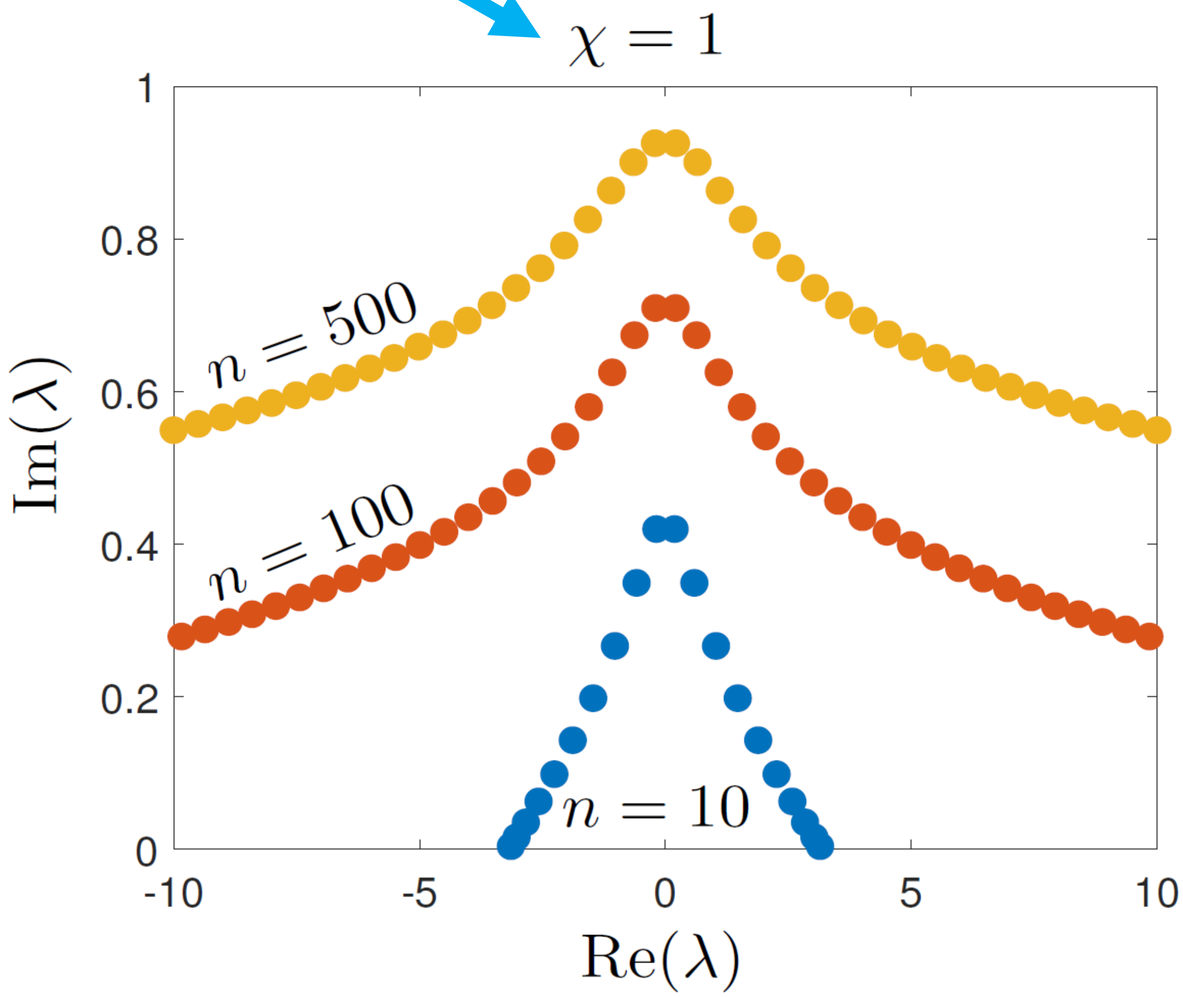
Resonant frequencies: $\lambda_k = \frac{\tan^{-1}(i\chi)}{2\pi} + \frac{k}{2}, \quad k \in \mathbb{Z}$

Discretized using FEM (n = discretization size)

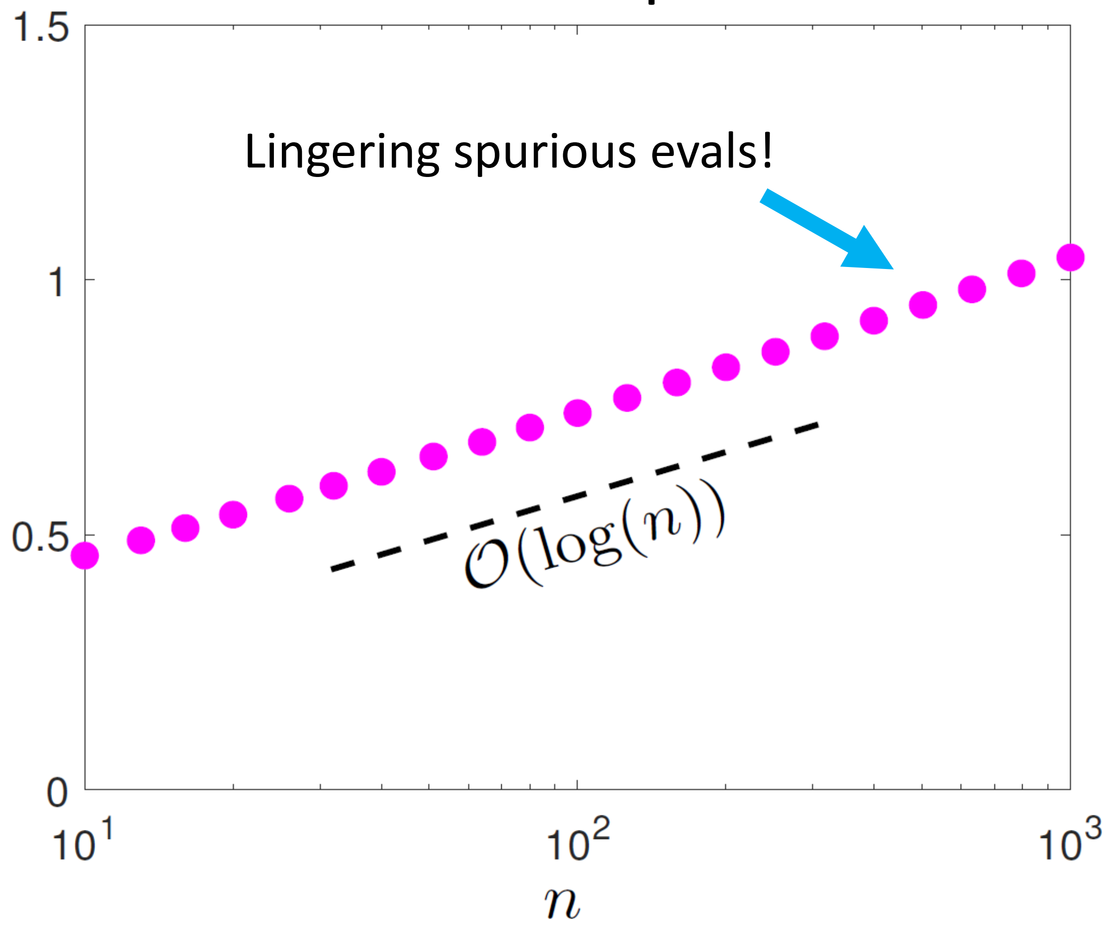
Example: One-dimensional acoustic wave

$$\lambda_k = \frac{\tan^{-1}(i\chi)}{2\pi} + \frac{k}{2}, \qquad k \in \mathbb{Z}$$

NLEVP default, **empty spectrum**!



Min abs of spurious λ

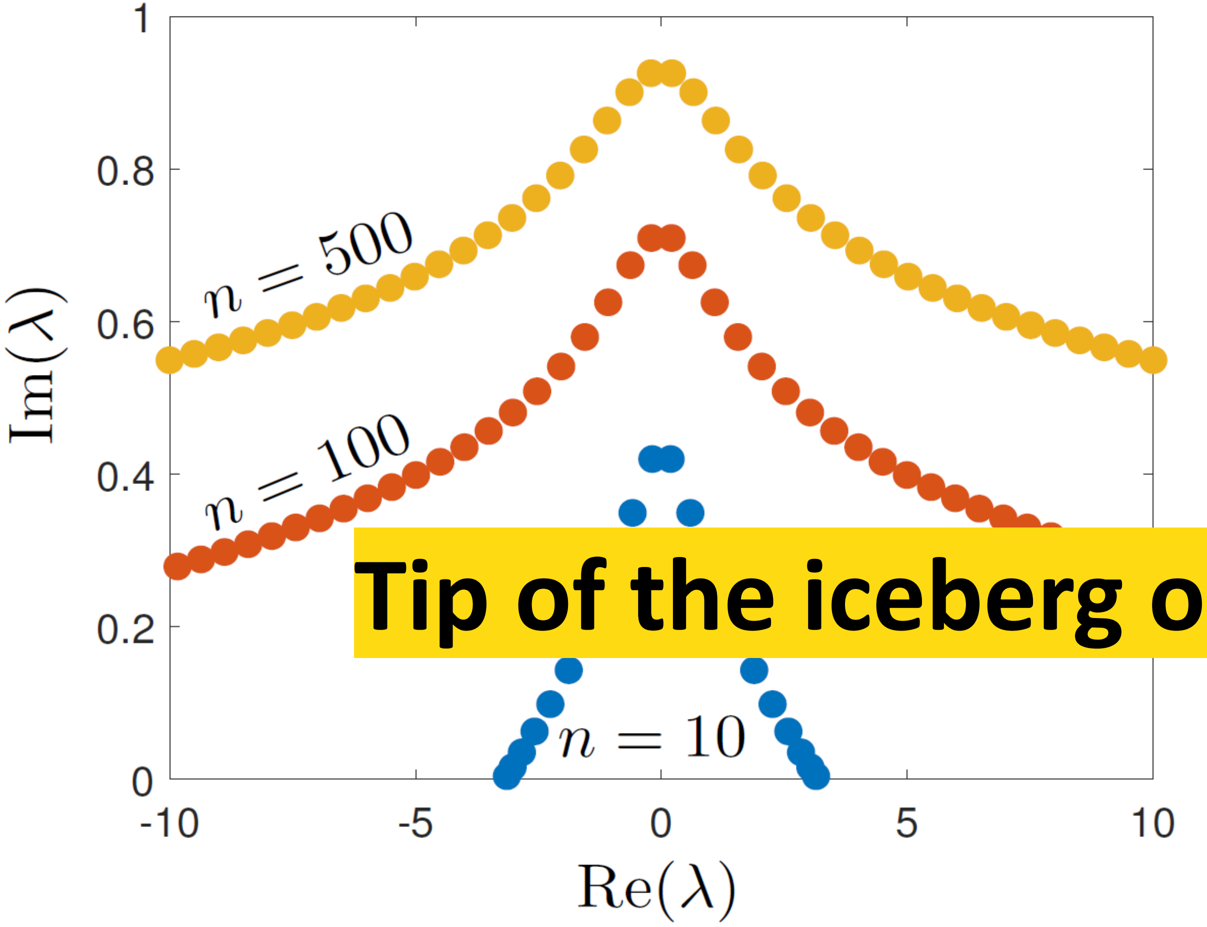


Example: One-dimensional acoustic wave

$$\lambda_k = \frac{\tan^{-1}(i\chi)}{2\pi} + \frac{k}{2}, \qquad k \in \mathbb{Z}$$

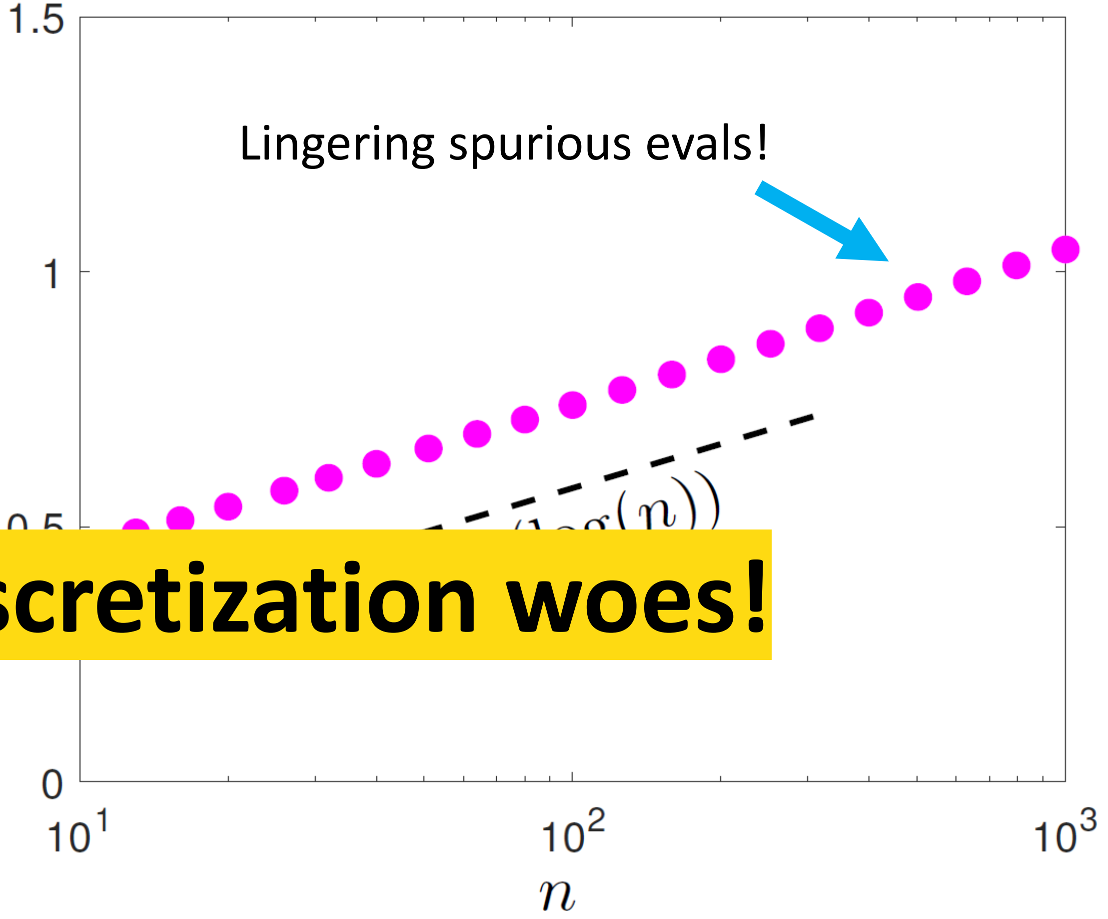
NLEVP default,
empty spectrum!

$\chi = 1$



Min abs of spurious λ

Lingering spurious evals!



Tip of the iceberg of discretization woes!

Discretization woes

Often, we discretize to a matrix NEP

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

Can cause serious issues:

- Spectral pollution (spurious eigenvalues).
- Spectral invisibility.
- Logarithmically 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. 

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

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

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

Stability of spectrum

Characterization through resolvent

Computational tool #1: Pseudospectra

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

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

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

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

Computational tool #1: Pseudospectra

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

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

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

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

$\mathcal{P}_n$: projection onto n-dimensional space

Assume: converge strongly to identity + an operator core condition

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

Computational tool #1: Pseudospectra

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

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

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

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

Rectangular sections

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

Folding

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

- 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.

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

Computational tool #1: Pseudospectra

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

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

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

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

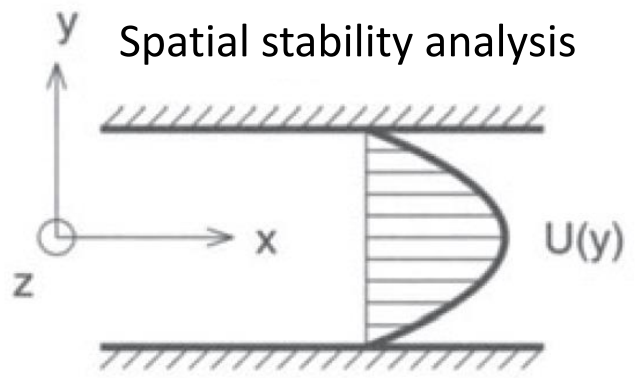
THEOREM: Let $\Gamma_n(T,\varepsilon) = \{\lambda \in \Omega: \gamma_n(\lambda) < \varepsilon\}$, then (in the Attouch-Wets metric)

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

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

Example of verification: Orr-Sommerfeld

Spatial stability analysis



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

$R = 5772.22, \omega = 0.264002$ ← Critical parameters

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

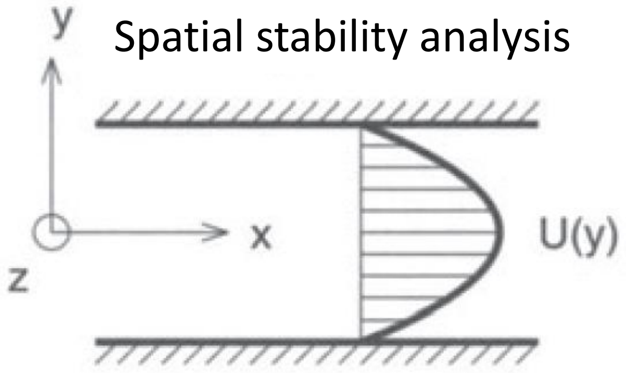
$$B(\lambda)\phi = -\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2} + \lambda^2\phi,\ \langle\phi,\psi\rangle = \int_{-1}^{1}\phi\bar{\psi} + \frac{d\phi}{dy}\overline{\frac{d\psi}{dy}}\mathrm{d}y,\ T(\lambda) = B(\lambda)^{-1}A(\lambda)$$

Example of verification: Orr-Sommerfeld

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

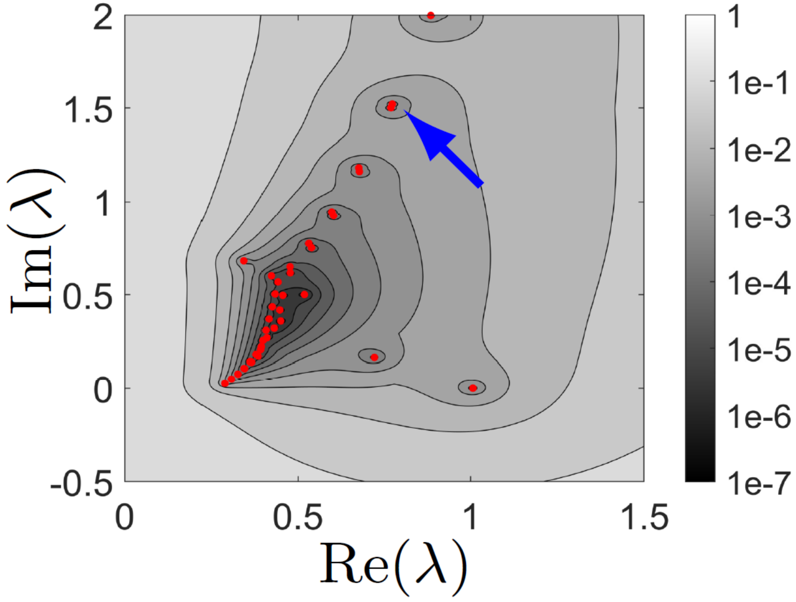
$R = 5772.22, \omega = 0.264002$

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

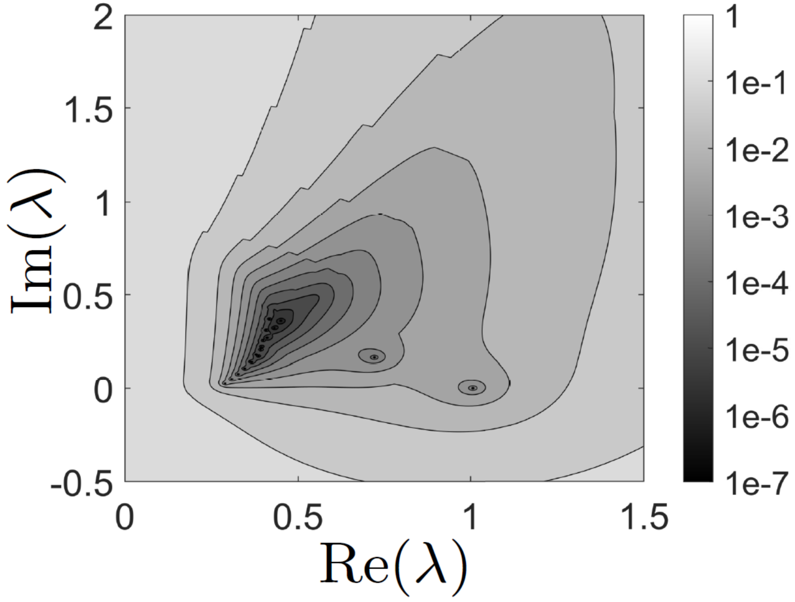


$\{\lambda \in \Omega: \gamma_n(\lambda) < \varepsilon\} \subset \mathrm{Sp}_\varepsilon(T)$

Cheb. Col., $n = 64$



$\gamma_n, n = 64$



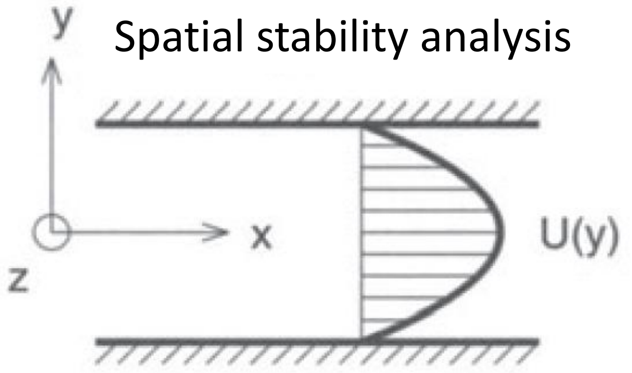
Which do we trust?

Example of verification: Orr-Sommerfeld

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

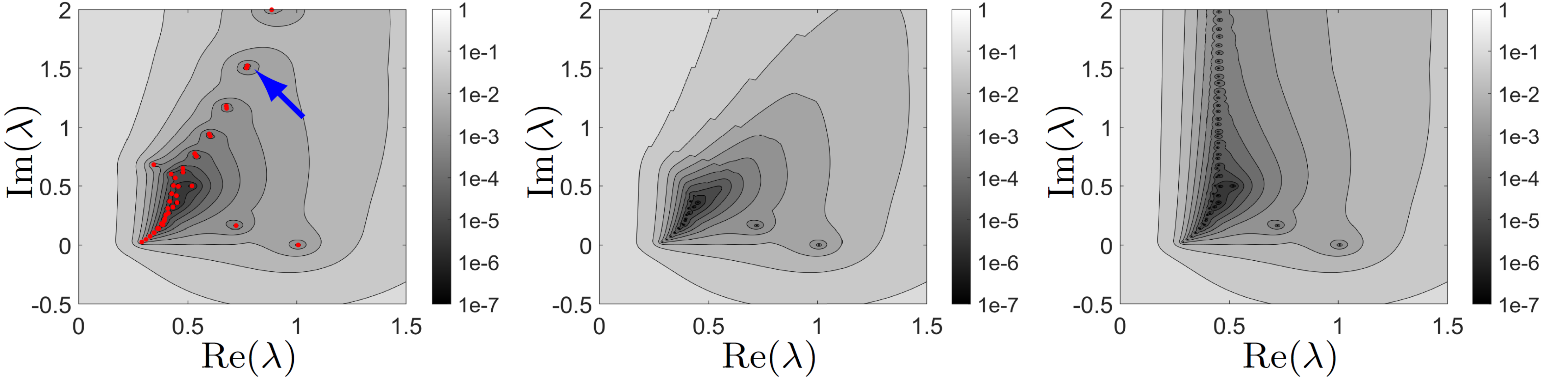
$R = 5772.22, \omega = 0.264002$

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



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

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

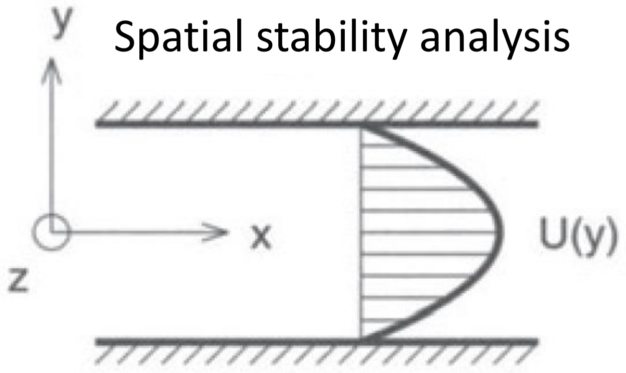


Example of verification: Orr-Sommerfeld

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

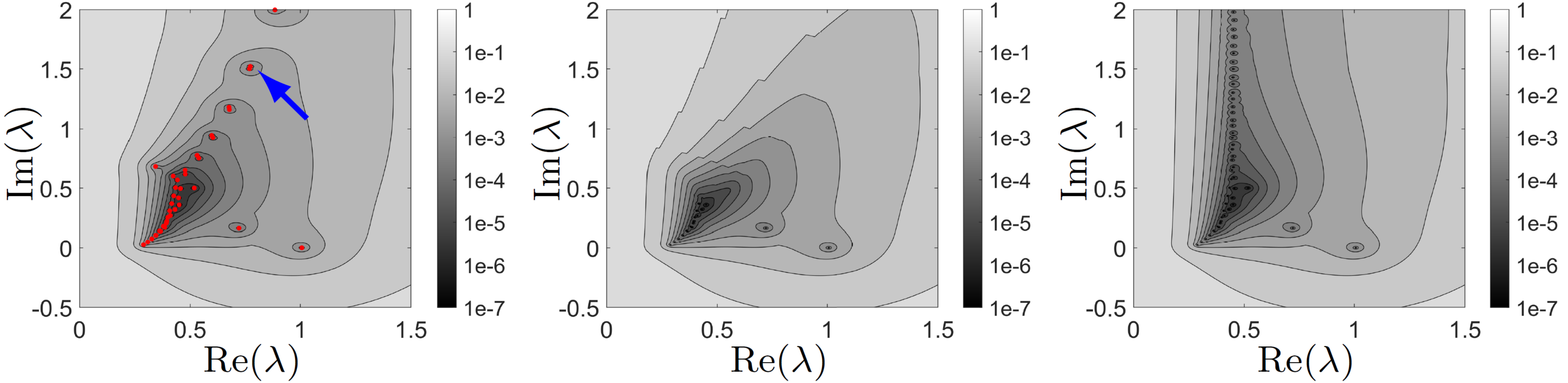
$R = 5772.22, \omega = 0.264002$

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



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

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: sum of all algebraic multiplicities of eigenvalues inside Ω.
- V & W: quasimatrices with m cols of right & left gen. eigenvectors.
- J: Jordan blocks.
- $R(z)$: 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.

Why is this so useful?

(1) Nonlinear $\longrightarrow$ linear.

Why is this so useful?

(1) Nonlinear $\longrightarrow$ linear.

(2) Infinite-dimensional $\longrightarrow$ finite-dimensional.

Why is this so useful?

(1) Nonlinear $\longrightarrow$ linear.

(2) Infinite-dimensional $\longrightarrow$ finite-dimensional.

(3) Computing spectra $\longrightarrow$ solving linear systems.

Why is this so useful?

(1) Nonlinear $\longrightarrow$ linear.

(2) Infinite-dimensional $\longrightarrow$ finite-dimensional.

(3) Computing spectra $\longrightarrow$ solving linear systems.

CANNOT OVERSTATE: Much easier for discretization to converge for solving linear systems than computing spectra!
This holds in theory and in practice.

InfBeyn algorithm

$\Gamma \subset \Omega$ contour enclosing m eigenvalues (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 via quadrature: $\tilde{A}_0, \tilde{A}_1$.

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

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

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

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 problems"*, 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: $L_1 = (VW^*)^\dagger, \;\; L_2 = (VW^*\mathcal{V}V_0)^\dagger$.

$$T(z)^{-1}L_1F(z) = -VW^*\mathcal{V}V_0 + R(z)L_1F(z)$$

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

$$F(z)L_2[T(z)^{-1} - R(z)] = -VW^*$$

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

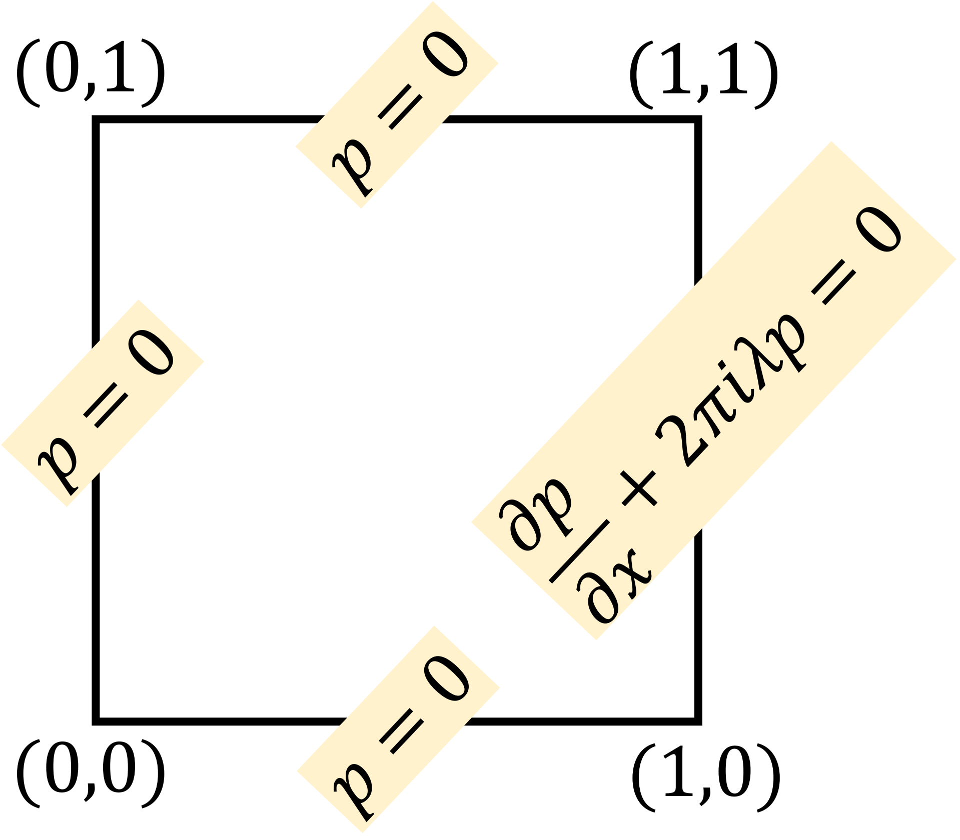
Use results from inf dim randomized NLA to bound terms with a $\mathcal{V}$.

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

Example: Two-dimensional acoustic wave

acoustic_wave_2d from NLEVP collection.

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + 4\pi^2\lambda^2 p = 0$$



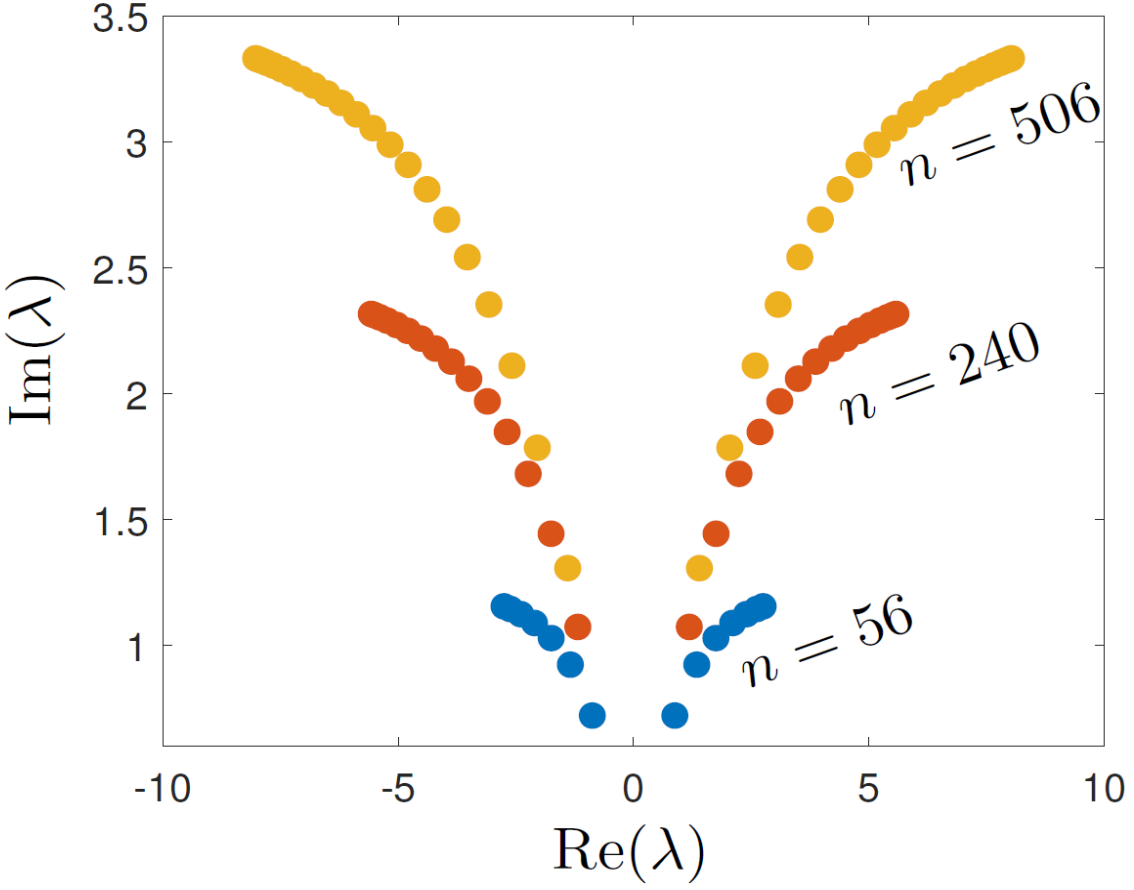
p corresponds to acoustic pressure.

λ correspond to resonant frequencies.

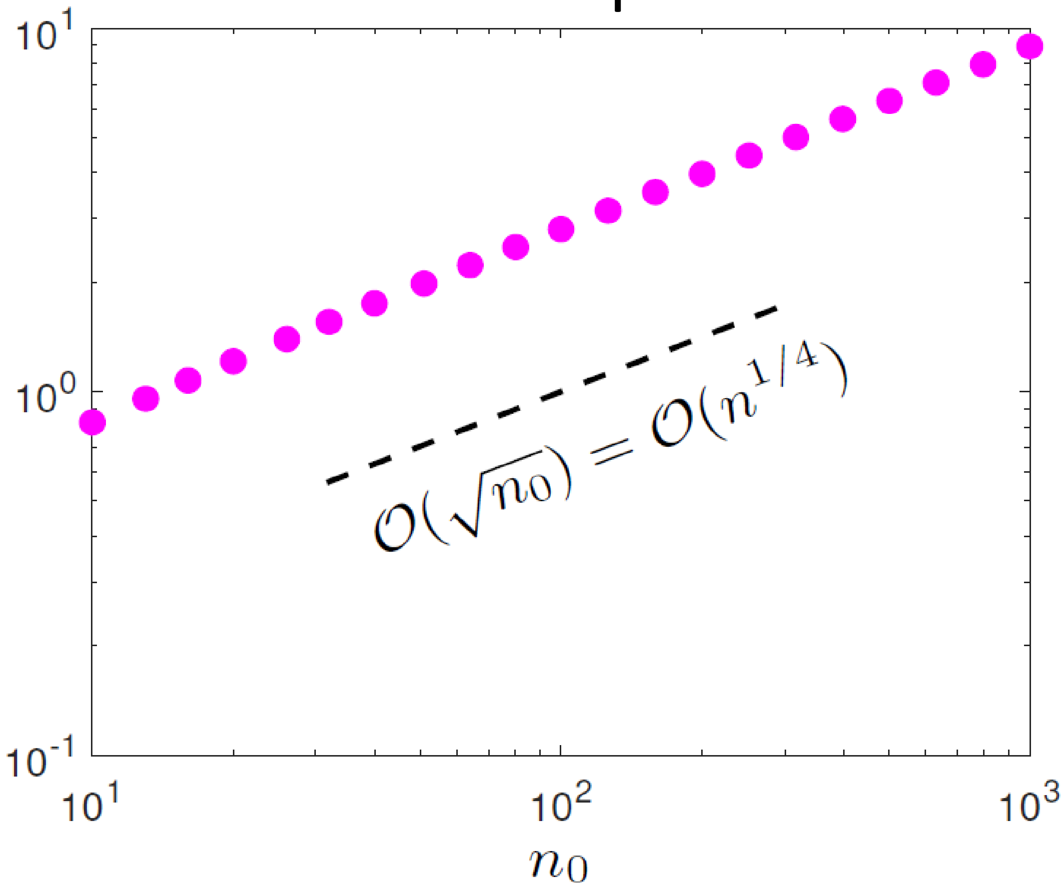
Discretized using FEM.

$(n = n_0(n_0 - 1)$ = discretization size).

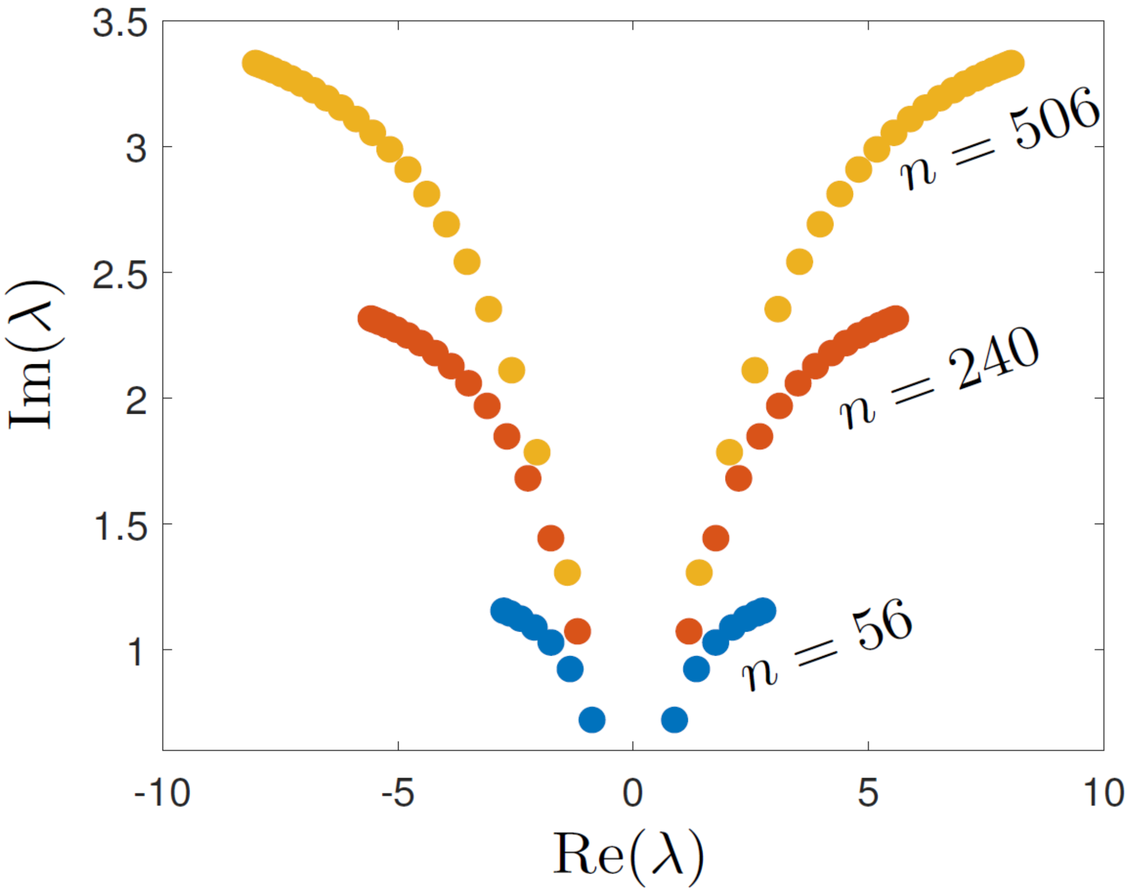
Example: Two-dimensional acoustic wave

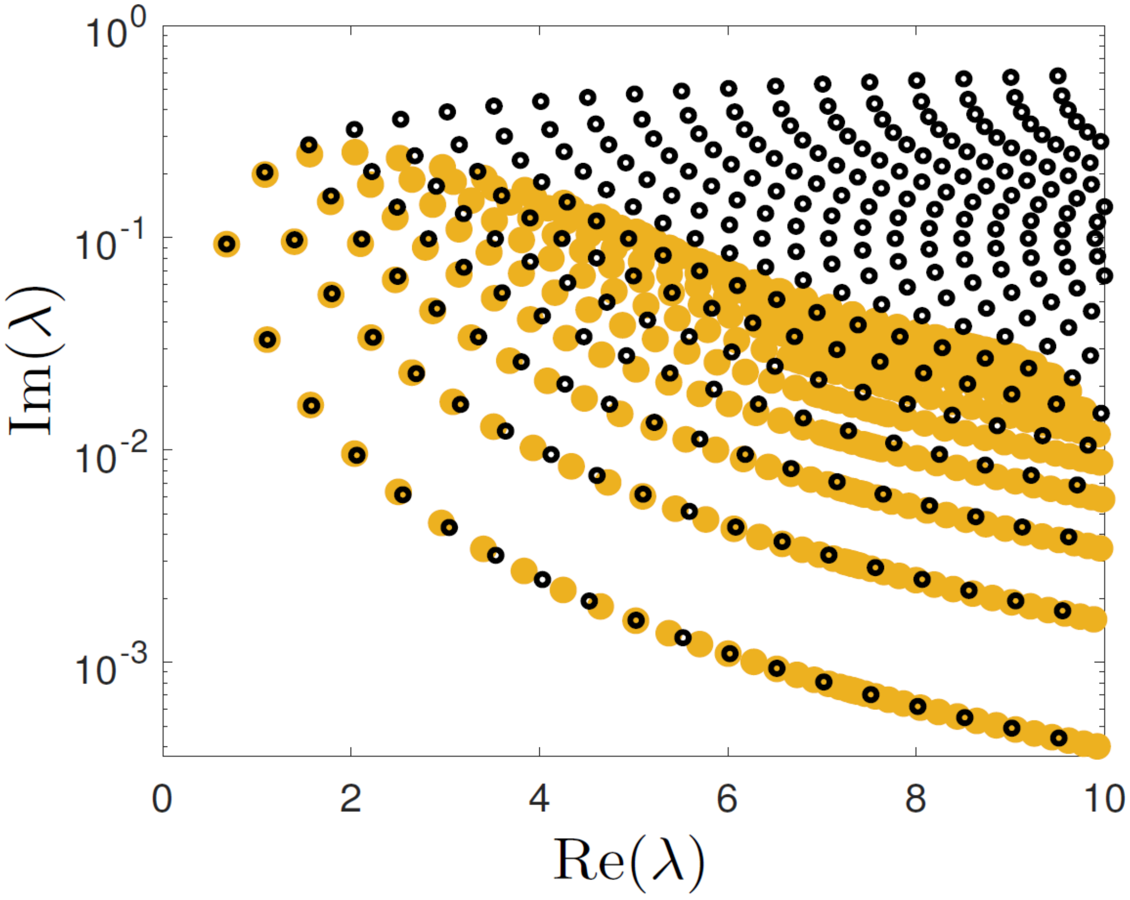


Min abs of spurious λ



Example: Two-dimensional acoustic wave



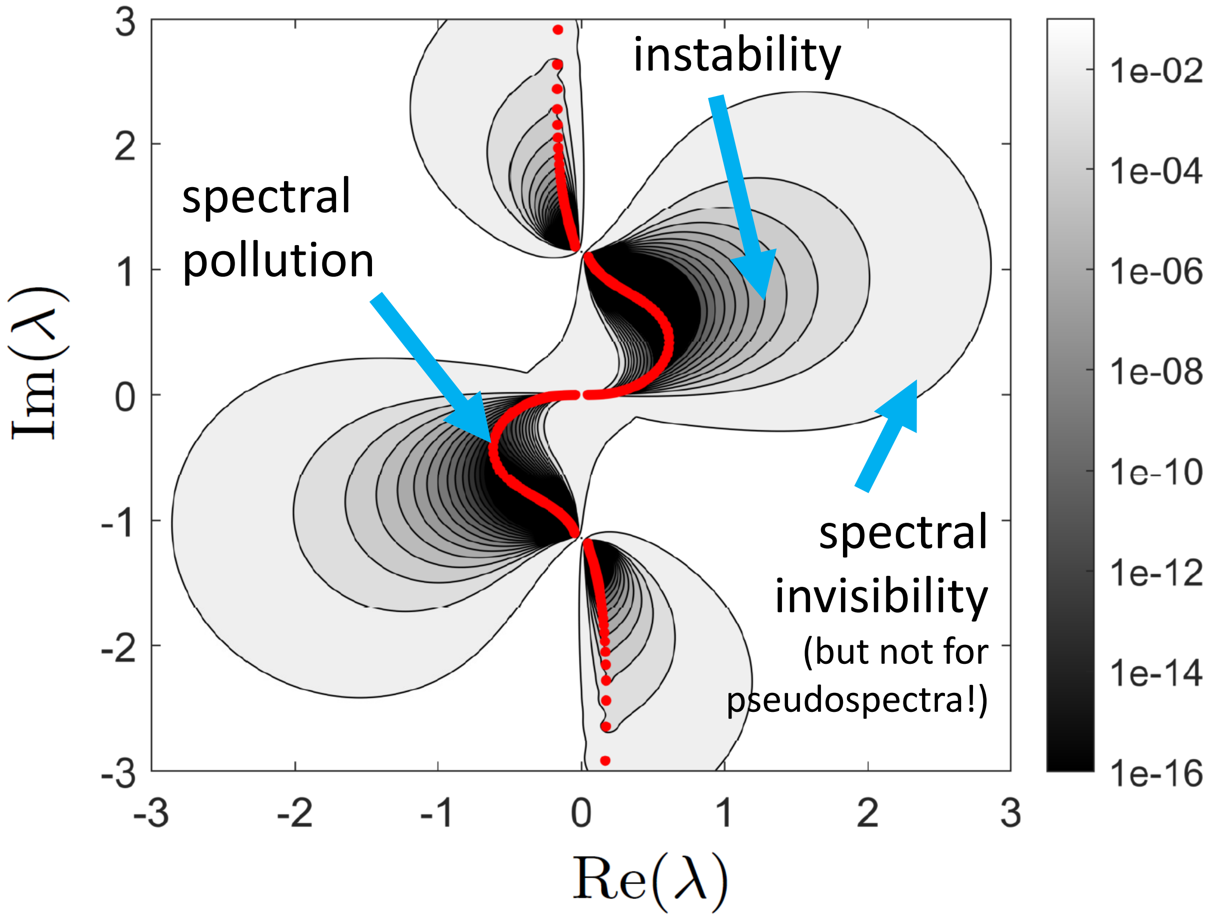


butterfly from NLEVP collection
$T(\lambda) = F(\lambda, S)$
S bilateral shift on $l^2(\mathbb{Z})$
F a rational function

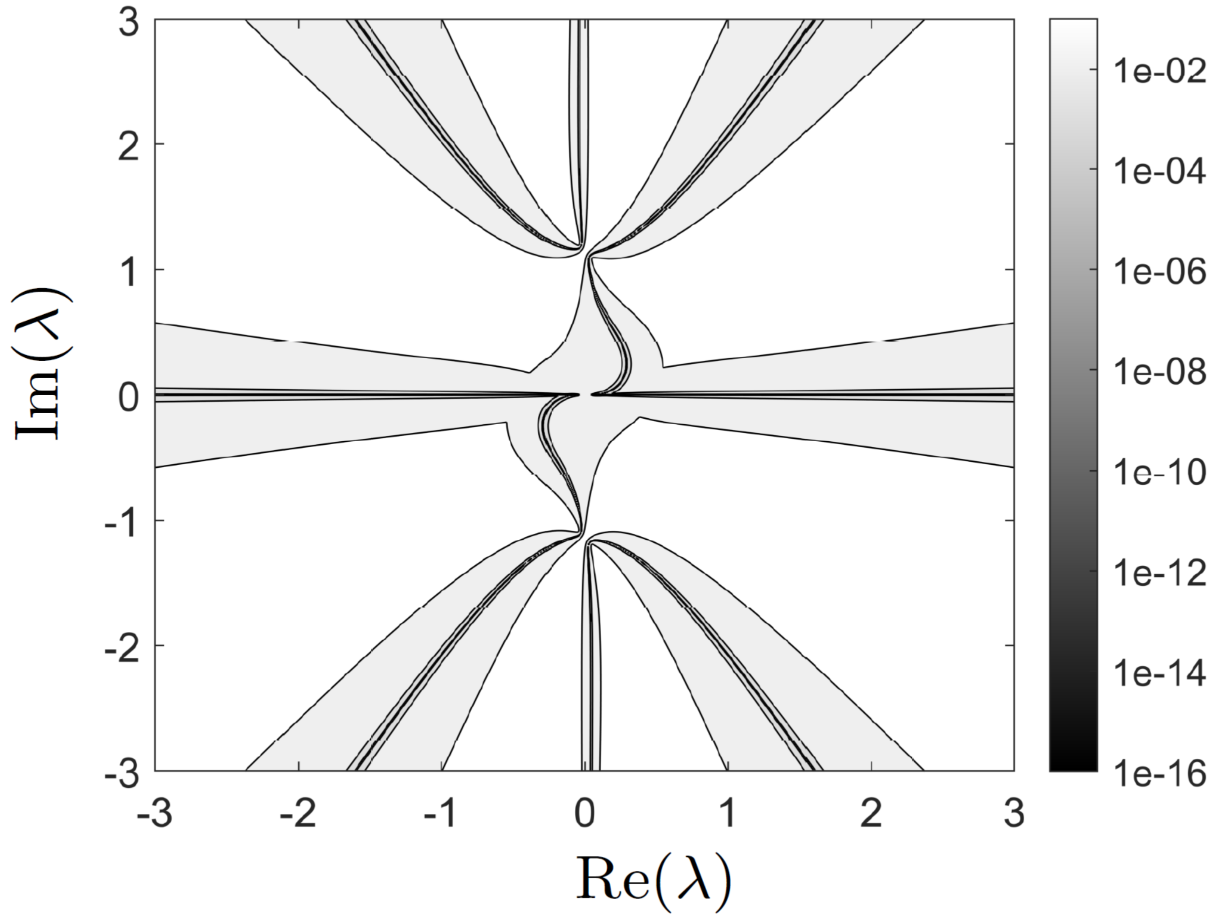
Example: Butterfly

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

Discretized $\mathcal{P}_n T(\lambda) \mathcal{P}_n^* \ (n = 500)$

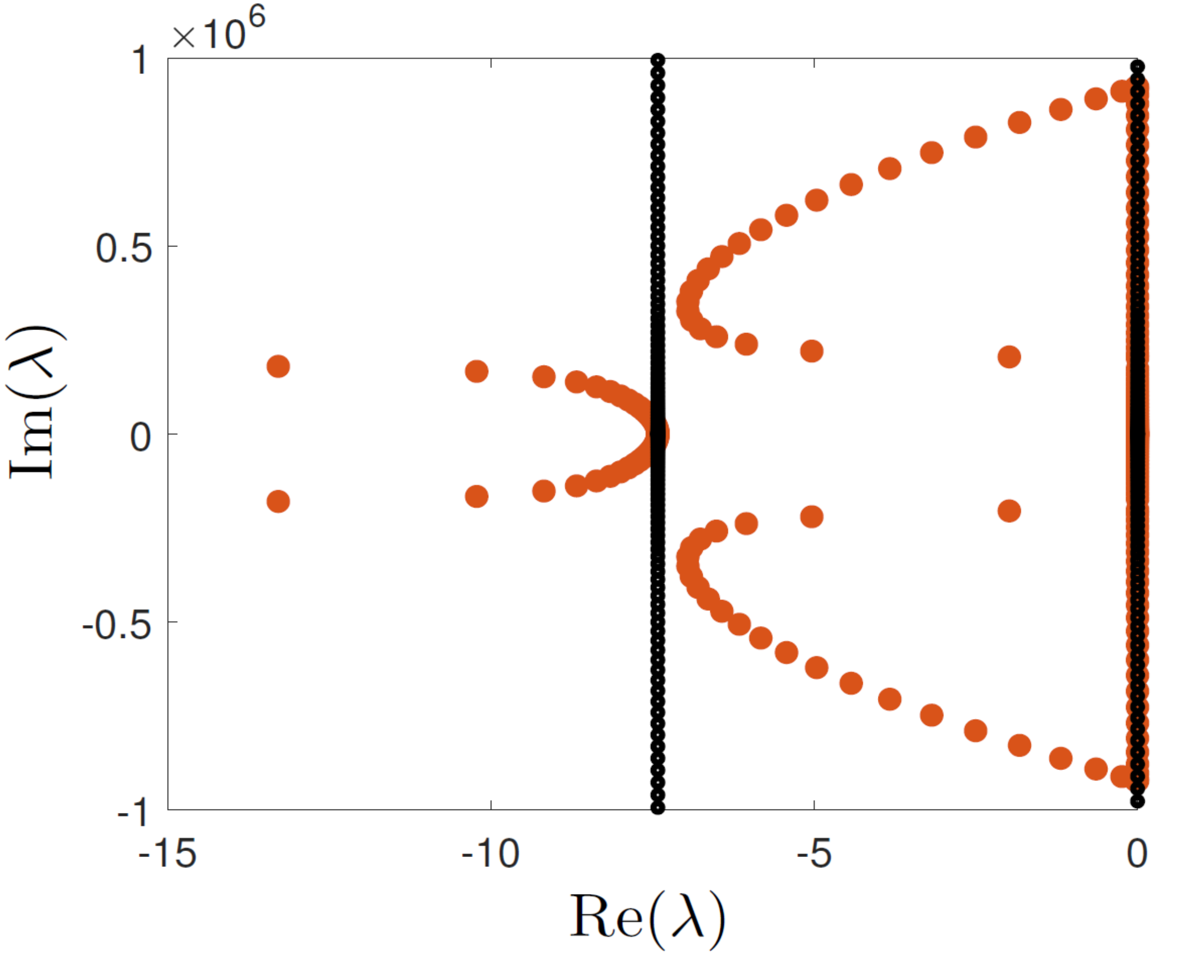


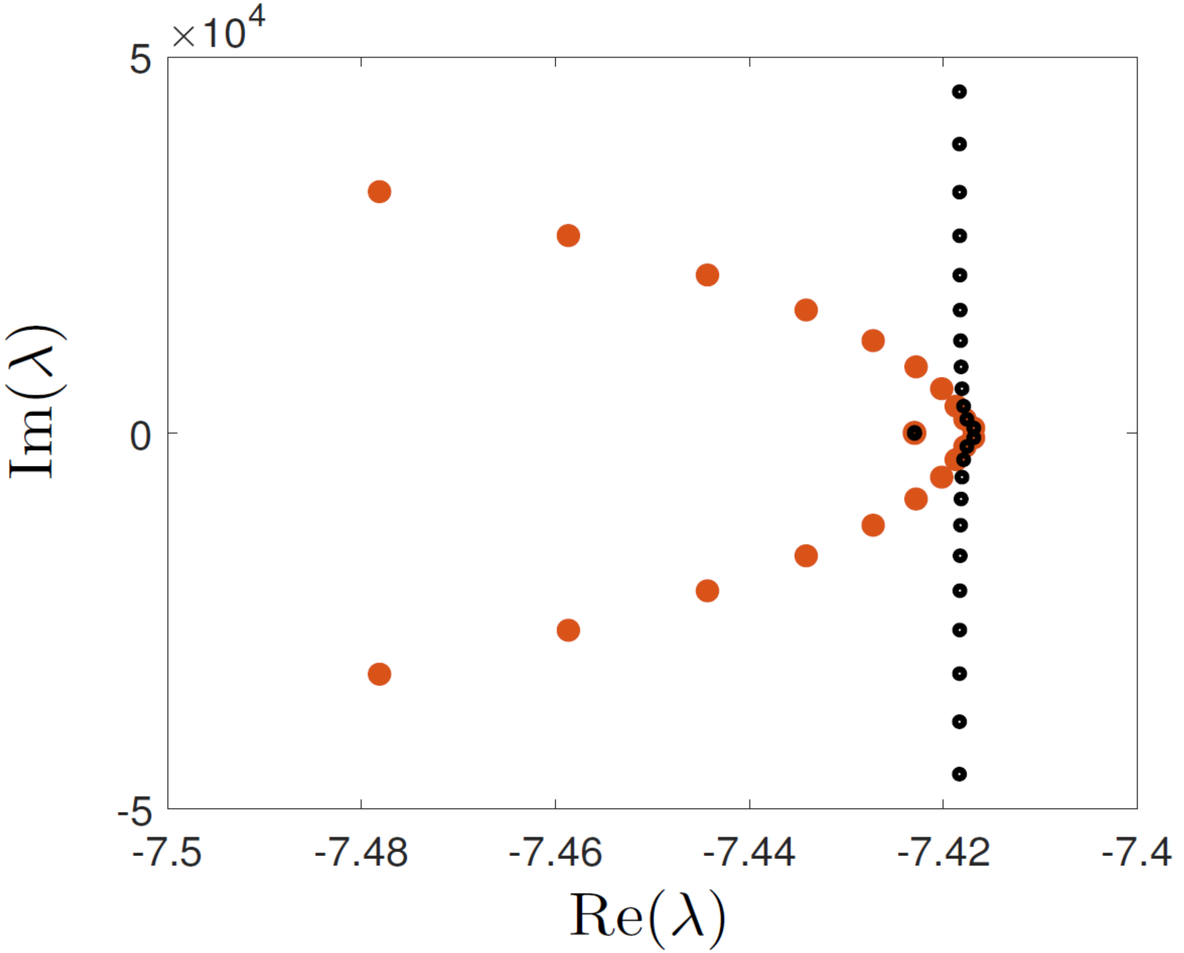
Method based on γ_n



Example: Damped beam

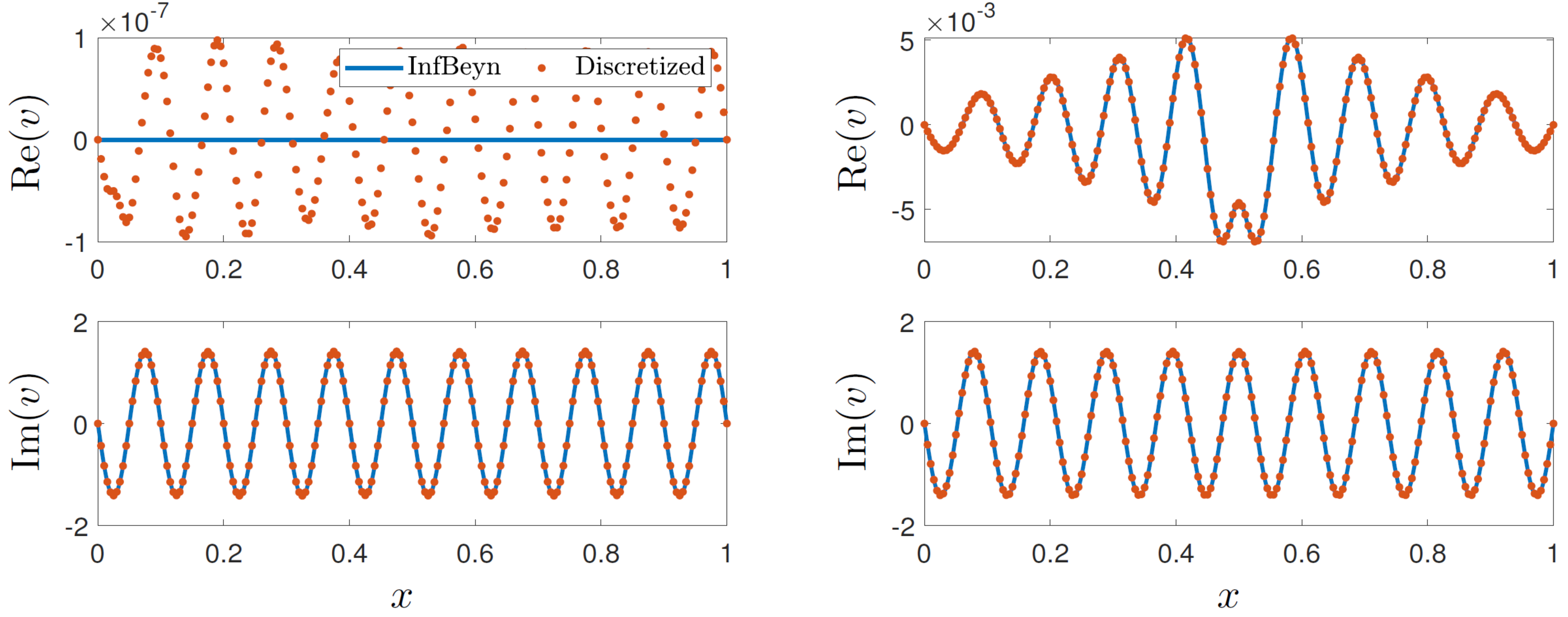
$$\frac{\mathrm{d}^4 v}{\mathrm{d}x^4} - \alpha\lambda^2 v = \beta\lambda\delta(x - 1/2)v, \qquad v(0) = v''(0) = v(1) = v''(1) = 0.$$





Example: Damped beam

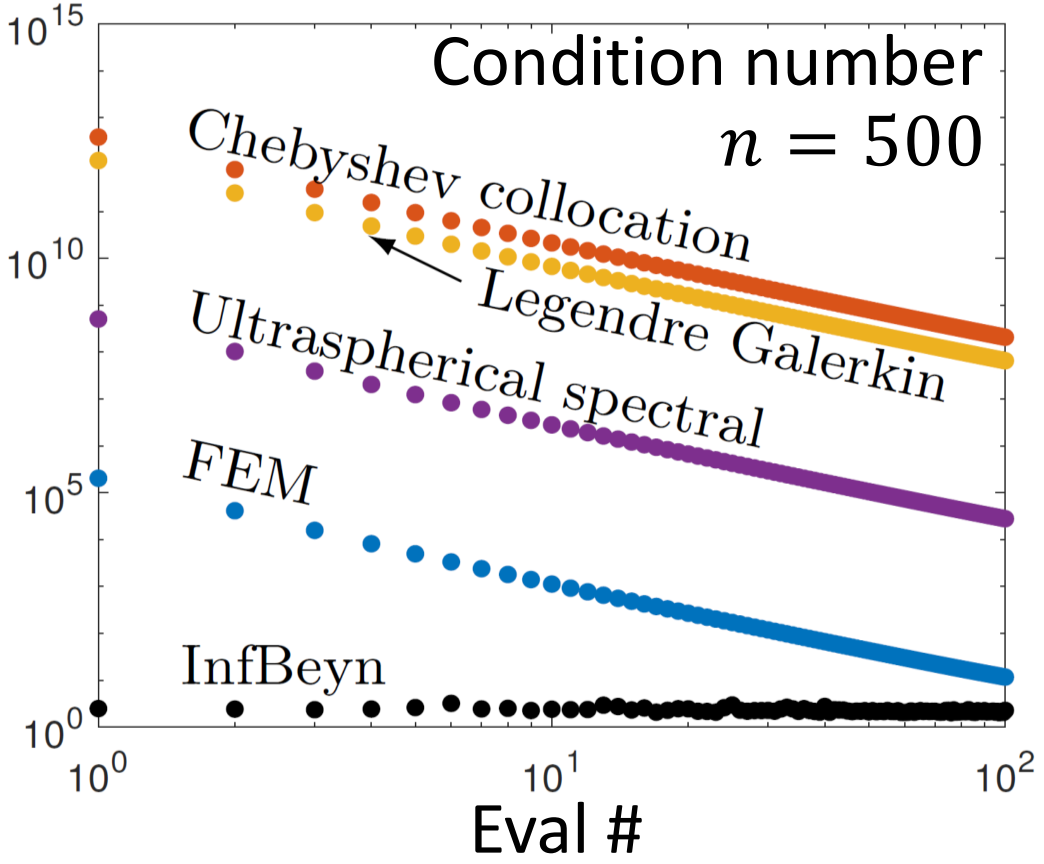
e-vector subspace error ≈ 0.001, e-val error ≈ 40 (InfBeyn error < 10^{-12})

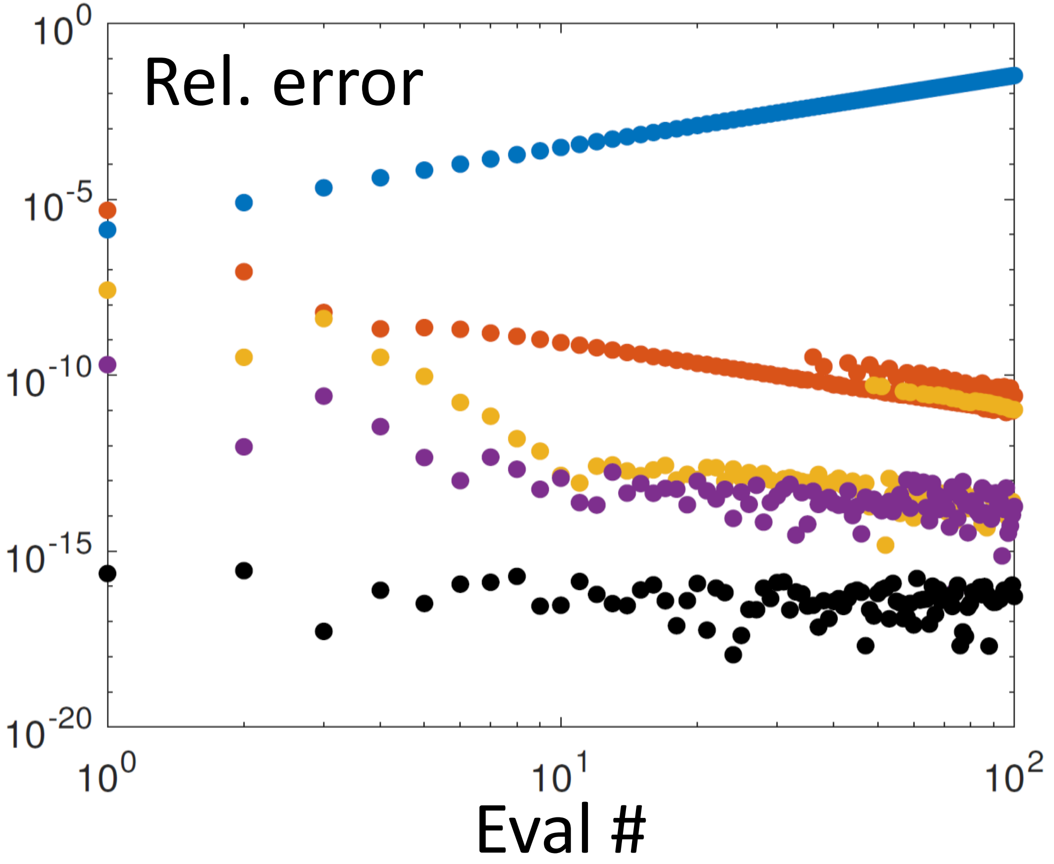


Example: Loaded string

damped_beam from NLEVP collection.

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





Example: Planar waveguide

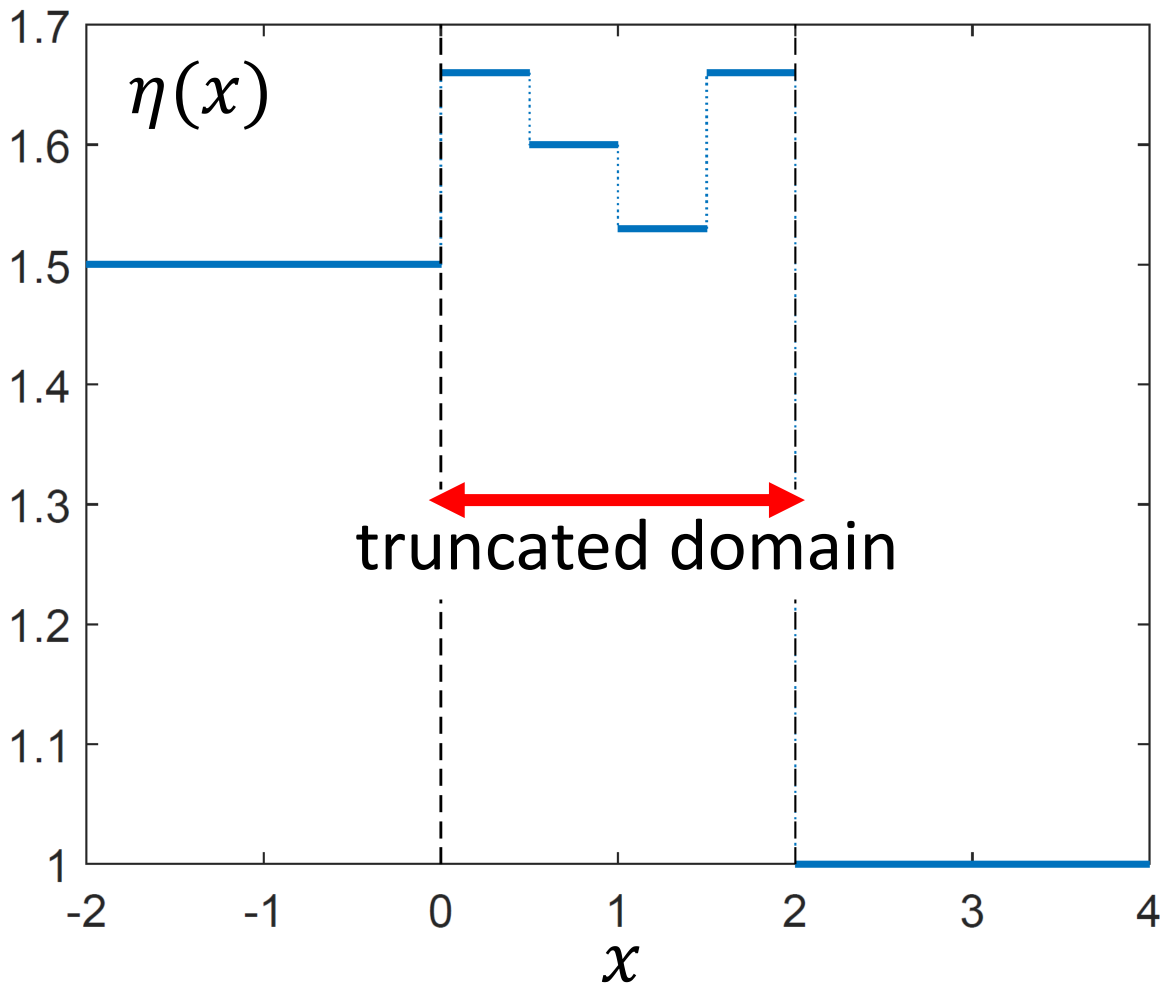
planar_waveguide from NLEVP collection.

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

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

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

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

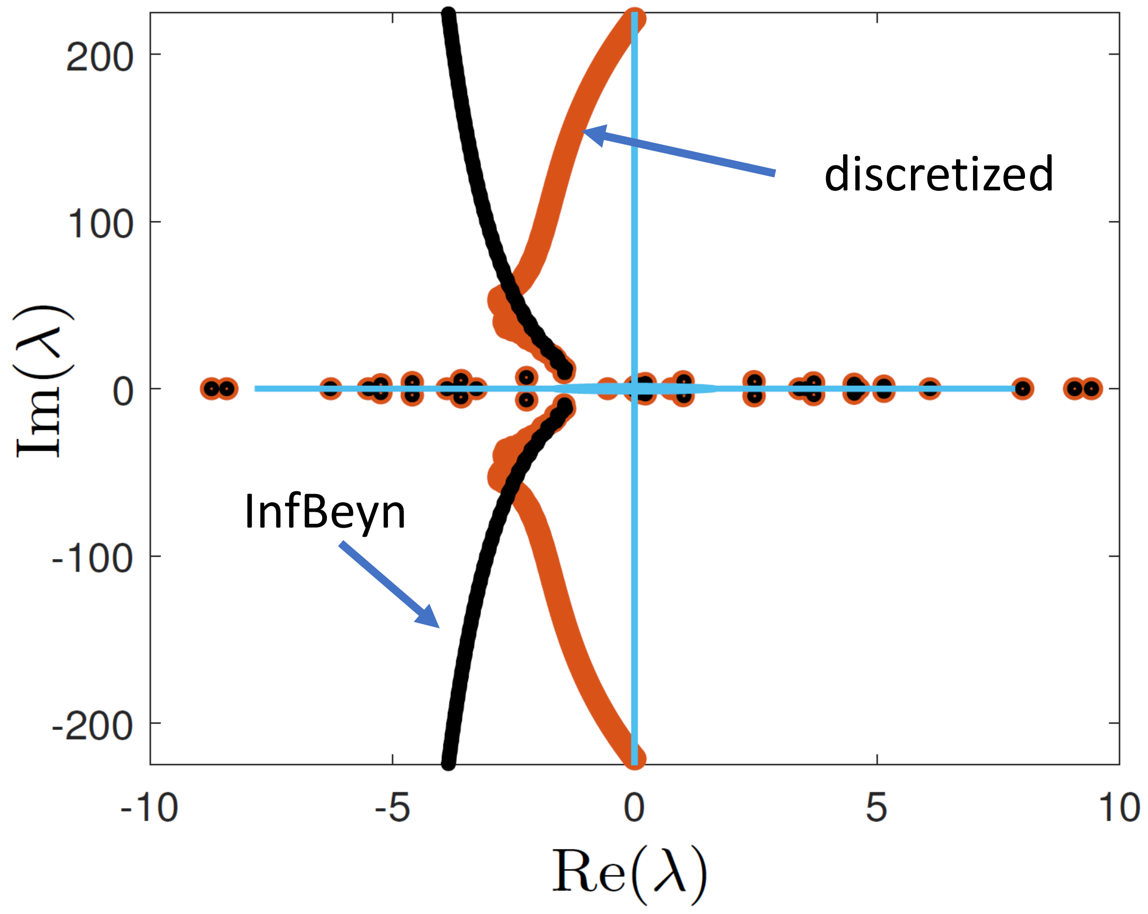


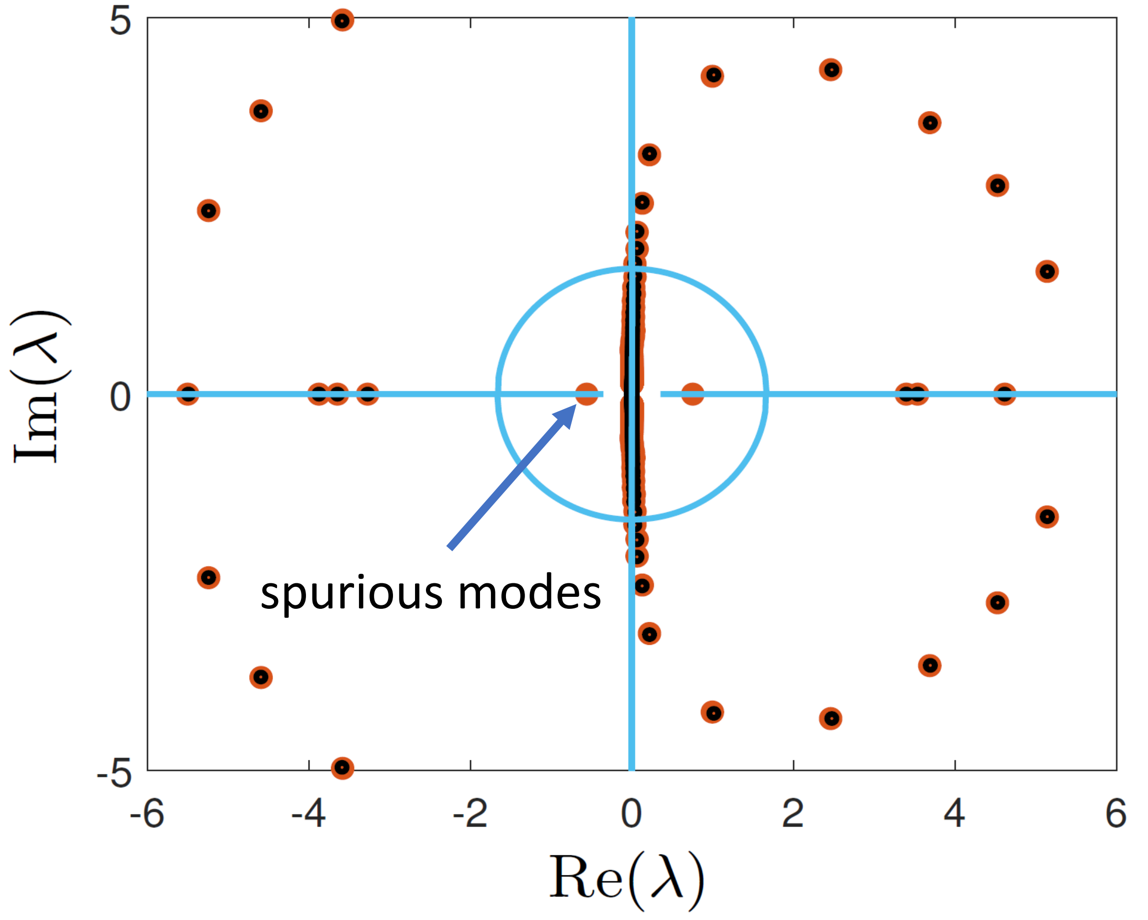
η corresponds to refractive index.

λ correspond to guided and leaky modes.

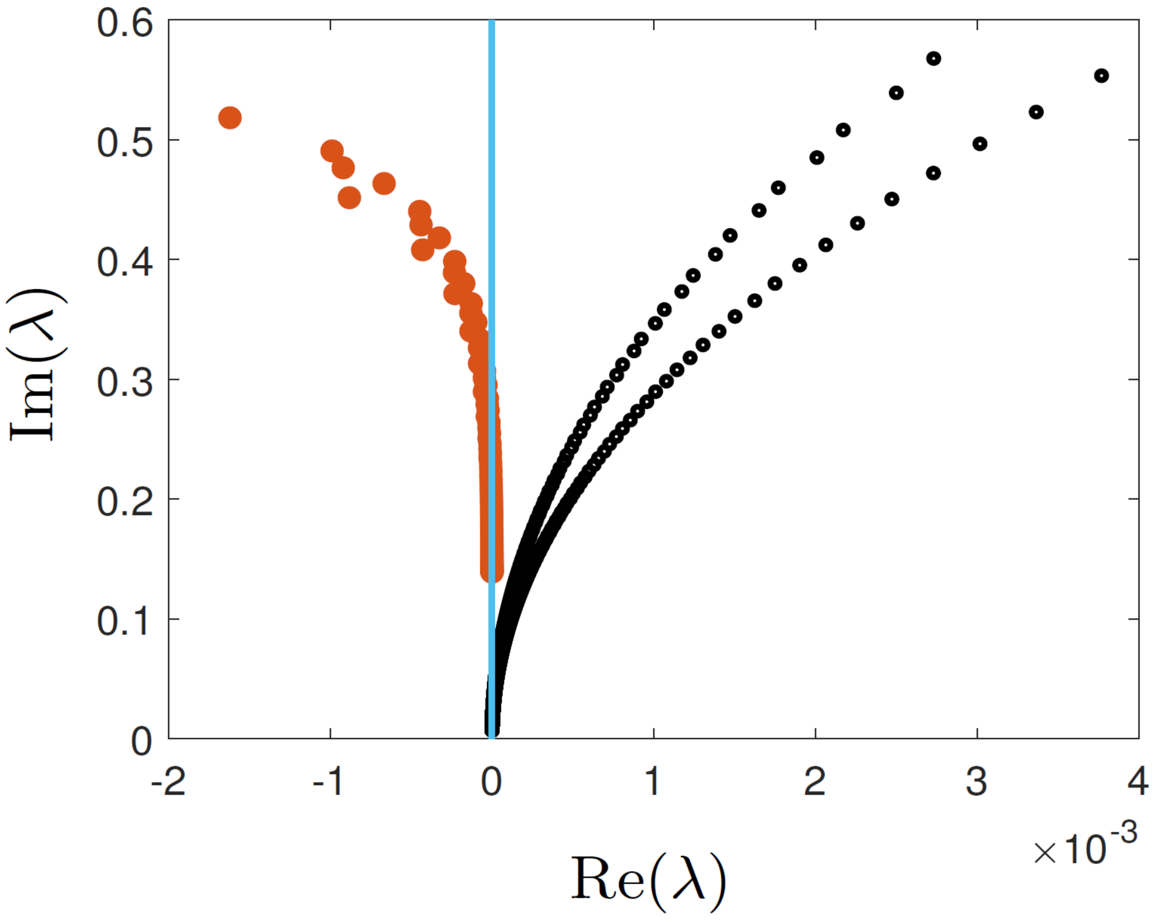
Discretized using FEM ($n = 129$, default)

Example: Planar waveguide

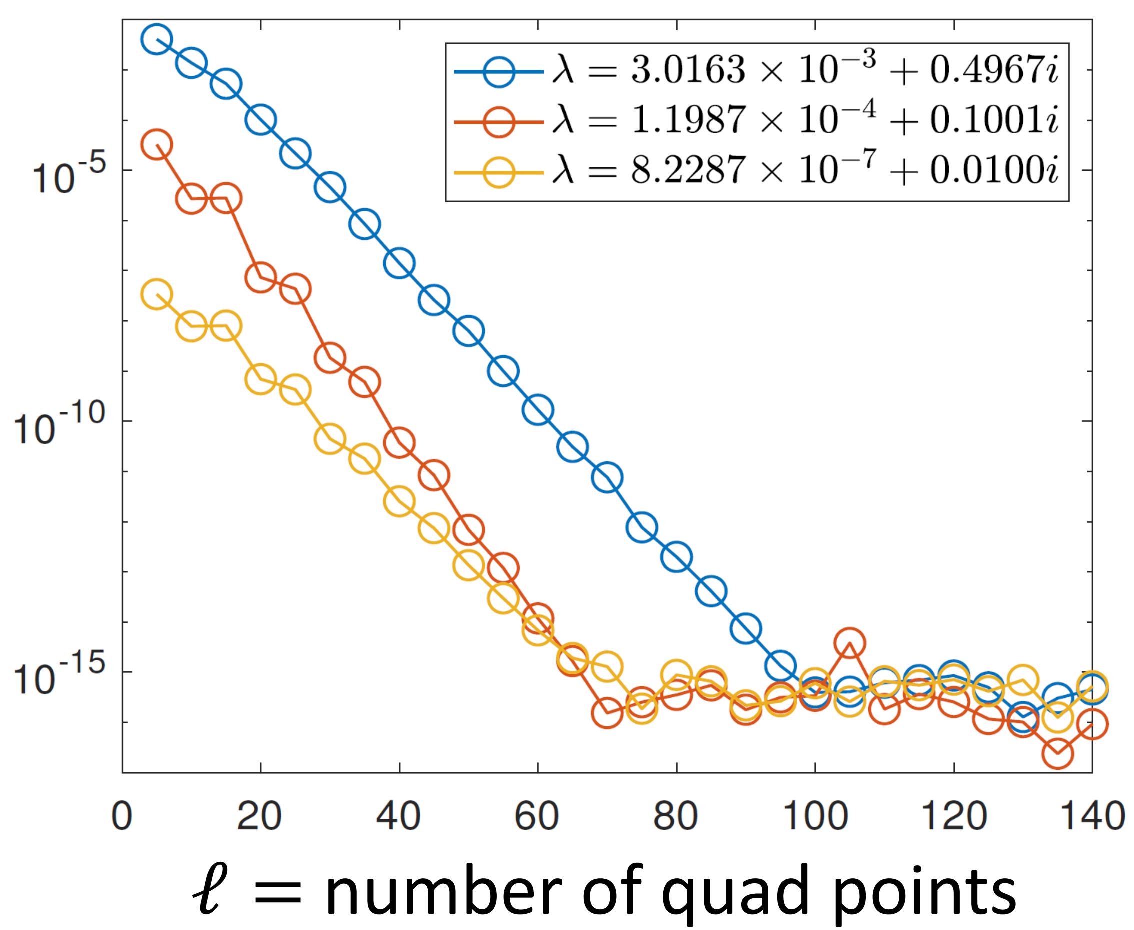




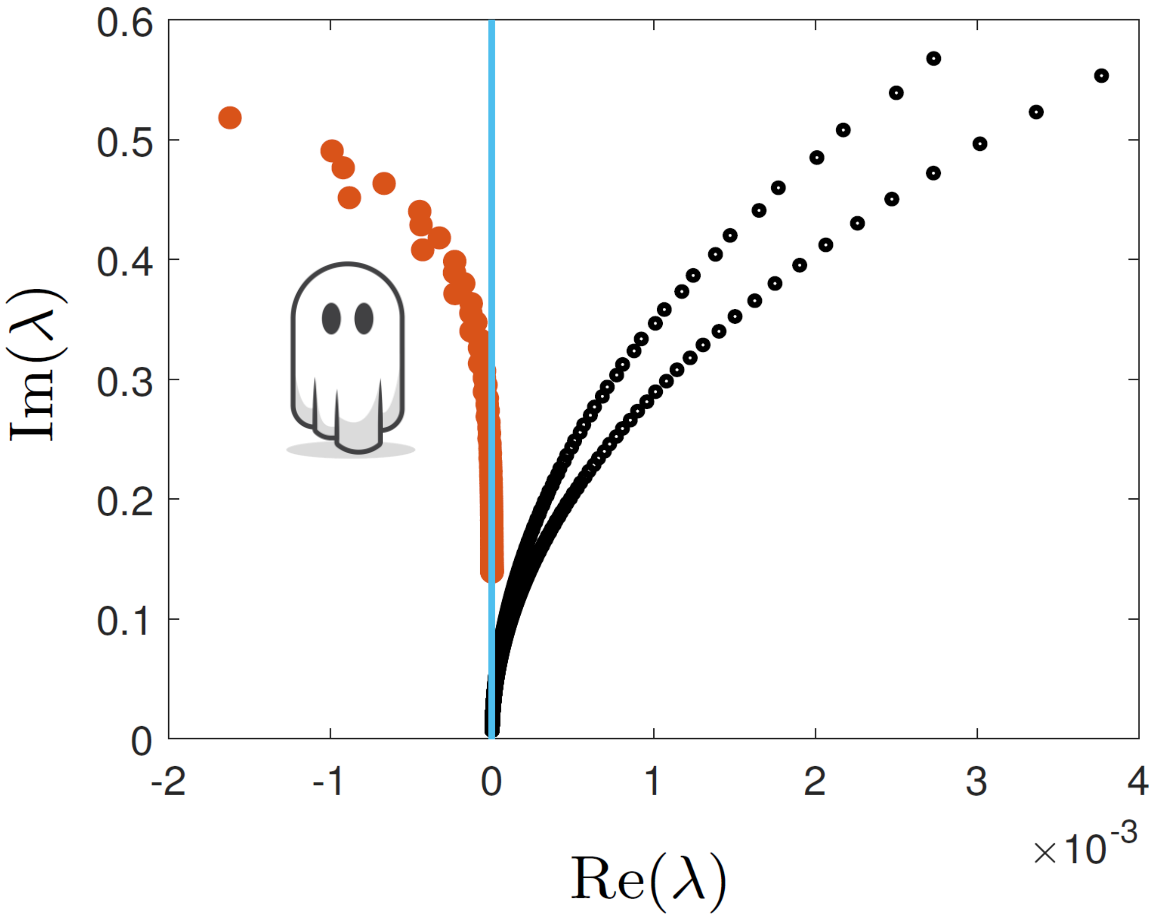
Example: Planar waveguide

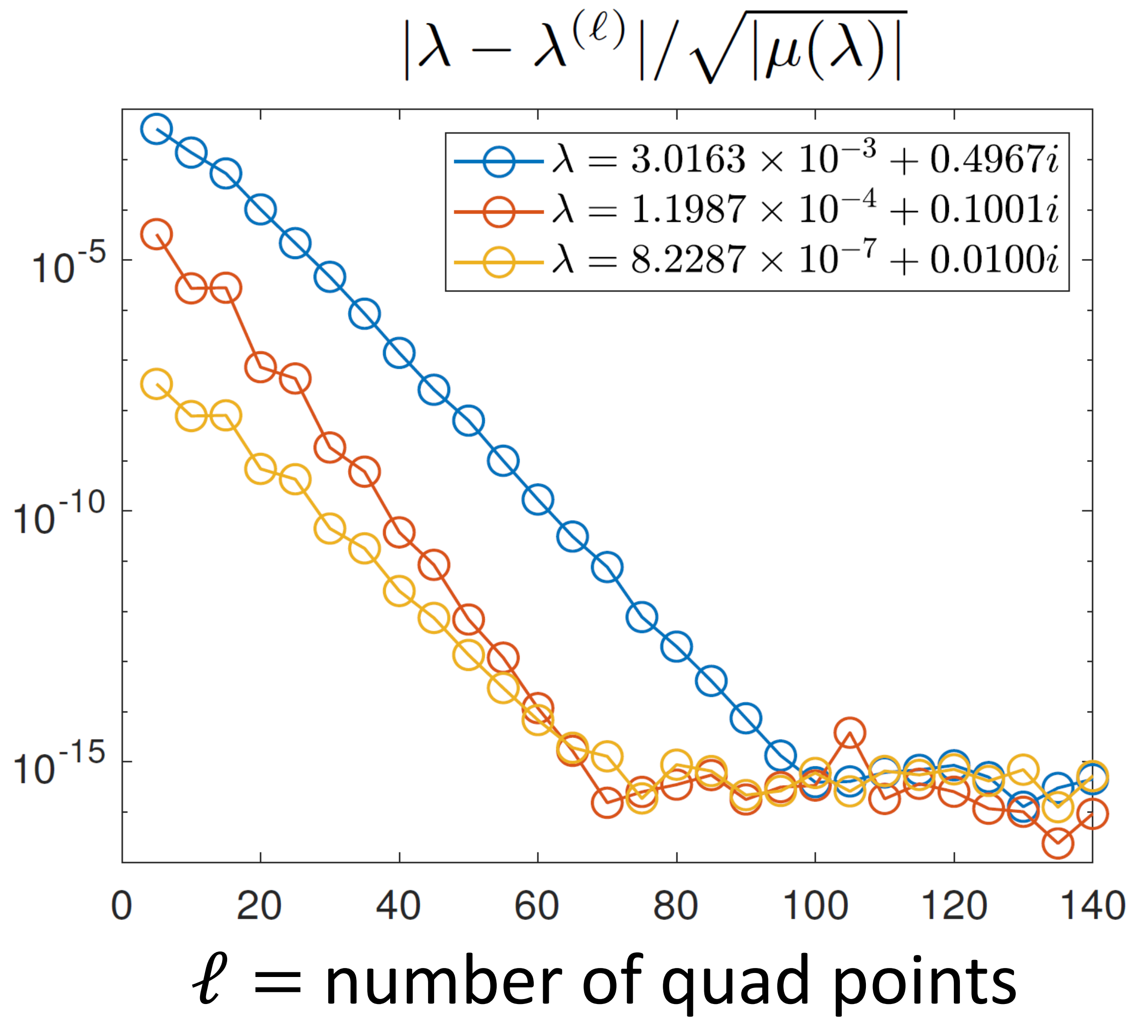


$|\lambda - \lambda^{(\ell)}| / \sqrt{|\mu(\lambda)|}$



Example: Planar waveguide

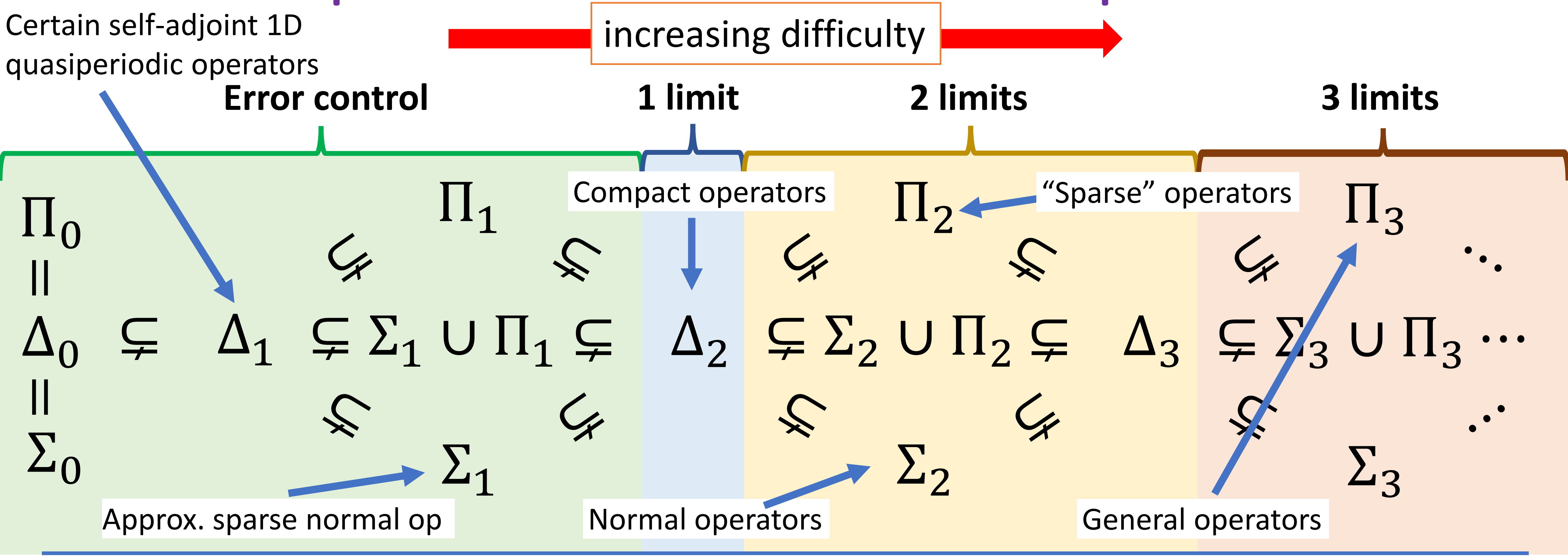




Bigger picture

- **Foundations:** Classify difficulty of computational problems.
  - Prove that algorithms are optimal (in any given computational model).
  - Find assumptions and methods for computational goals.
- 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.

Sample: some results for linear problems



- C., "*The foundations of infinite-dimensional spectral computations,*" **PhD diss.**, University of Cambridge, 2020.
- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "*On the solvability complexity index hierarchy and towers of algorithms,*" preprint.
- C., Horning, Townsend, "*Computing spectral measures of self-adjoint operators,*" **SIAM Rev.**, 2021.
- Ben-Artzi, Marletta, Rösler, "*Computing the sound of the sea in a seashell,*" **Found. Comput. Math.**, 2022.
- Ben-Artzi, Marletta, Rösler, "*Computing scattering resonances,*" **J. Eur. Math. Soc.**, 2022.
- C., "*On the computation of geometric features of spectra of linear operators on Hilbert spaces,*" **Found. Comput. Math.**, 2022.
- Webb, Olver, "*Spectra of Jacobi operators via connection coefficient matrices,*" **Commun. Math. Phys.**, 2021.
- Rösler, Stepanenko, "*Computing eigenvalues of the Laplacian on rough domains,*" preprint.
- Rösler, Tretter, "*Computing Klein-Gordon Spectra,*" prepint.

Summary for NEPs

- Discretization can cause serious issues.
- **InfBeyn** overcomes these in regions of discrete spectra: **convergent, stable, efficient**.
- Compute pseudospectra with explicit **error control** (generic pencils, even with essential spectra!)

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

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 problems"*, preprint.

References

[1] Colbrook, Matthew J., and Alex Townsend. "Avoiding discretization issues for nonlinear eigenvalue problems." arXiv preprint arXiv:2305.01691 (2023).

[2] Colbrook, Matthew J. "Computing semigroups with error control." SIAM Journal on Numerical Analysis 60.1 (2022): 396-422.

[3] Colbrook, Matthew J., and Lorna J. Ayton. "A contour method for time-fractional PDEs and an application to fractional viscoelastic beam equations." Journal of Computational Physics 454 (2022): 110995.

[4] Colbrook, Matthew. The foundations of infinite-dimensional spectral computations. Diss. University of Cambridge, 2020.

[5] Ben-Artzi, J., Colbrook, M. J., Hansen, A. C., Nevanlinna, O., & Seidel, M. (2020). Computing Spectra--On the Solvability Complexity Index Hierarchy and Towers of Algorithms. arXiv preprint arXiv:1508.03280.

[6] Colbrook, Matthew J., Vegard Antun, and Anders C. Hansen. "The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem." Proceedings of the National Academy of Sciences 119.12 (2022): e2107151119.

[7] Colbrook, Matthew, Andrew Horning, and Alex Townsend. "Computing spectral measures of self-adjoint operators." SIAM review 63.3 (2021): 489-524.

[8] Colbrook, Matthew J., Bogdan Roman, and Anders C. Hansen. "How to compute spectra with error control." Physical Review Letters 122.25 (2019): 250201.

[9] Colbrook, Matthew J., and Anders C. Hansen. "The foundations of spectral computations via the solvability complexity index hierarchy." Journal of the European Mathematical Society (2022).

[10] Colbrook, Matthew J. "Computing spectral measures and spectral types." Communications in Mathematical Physics 384 (2021): 433-501.

[11] Colbrook, Matthew J., and Anders C. Hansen. "On the infinite-dimensional QR algorithm." Numerische Mathematik 143 (2019): 17-83.

[12] Colbrook, Matthew J. "On the computation of geometric features of spectra of linear operators on Hilbert spaces." Foundations of Computational Mathematics (2022): 1-82.

[13] Colbrook, Matthew. "Pseudoergodic operators and periodic boundary conditions." Mathematics of Computation 89.322 (2020): 737-766.

[14] Colbrook, Matthew J., and Alex Townsend. "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems." arXiv preprint arXiv:2111.14889 (2021).

[15] Colbrook, Matthew J., Lorna J. Ayton, and Máté Szőke. "Residual dynamic mode decomposition: robust and verified Koopmanism." Journal of Fluid Mechanics 955 (2023): A21.

[16] Colbrook, Matthew J. "The mpEDMD algorithm for data-driven computations of measure-preserving dynamical systems." SIAM Journal on Numerical Analysis 61.3 (2023): 1585-1608.

[17] Johnstone, Dean, et al. "Bulk localized transport states in infinite and finite quasicrystals via magnetic aperiodicity." Physical Review B 106.4 (2022): 045149.

[18] Colbrook, Matthew J., et al. "Computing spectral properties of topological insulators without artificial truncation or supercell approximation." IMA Journal of Applied Mathematics 88.1 (2023): 1-42.

[19] Colbrook, Matthew J., and Andrew Horning. "Specsolve: spectral methods for spectral measures." arXiv preprint arXiv:2201.01314 (2022).

[20] Colbrook, Matthew, Andrew Horning, and Alex Townsend. "Resolvent-based techniques for computing the discrete and continuous spectrum of differential operators." XXI Householder Symposium on Numerical Linear Algebra. 2020.

[21] Brunton, Steven L., and Matthew J. Colbrook. "Resilient Data-driven Dynamical Systems with Koopman: An Infinite-dimensional Numerical Analysis Perspective."