

FoCM: Solve-the-discretize for NLEPS

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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

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

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

 $Sp(T) = \{\lambda \in \Omega: T(\lambda) \text{ is not invertible}\}$ $Sp_d(T) = \{\lambda \in Sp(T): \lambda \text{ isolated}, T(\lambda) \text{ Fredholm}\}$ $Sp_{ess}(T) = Sp(T) \setminus Sp_d(T)$

* 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

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

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.



Stability of spectrum

Characterization through resolvent

Computational tool #1: Pseudospectra

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

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

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

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

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

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Computational tool #1: Pseudospectra $\mathcal{A}(\varepsilon) = \left\{ E: \Omega \to \mathcal{B}(\mathcal{H}) \text{ holomorphic: } \sup_{\lambda \in \Omega} \| E(\lambda) \| < \varepsilon \right\}$ $\operatorname{Sp}_{\varepsilon}(T) = \left(\int \operatorname{Sp}(T+E) = \{\lambda \in \Omega : \|T(\lambda)^{-1}\|^{-1} < \varepsilon \}$ $E \in \mathcal{A}(\varepsilon)$ **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** Folding $\sigma_{\inf}(\mathcal{P}_{f(n)}T(\lambda)\mathcal{P}_n^*)$ $\sqrt{\sigma_{\inf}(\mathcal{P}_n T(\lambda)^* T(\lambda) \mathcal{P}_n^*)}$

- 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.

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THEOREM: Let $\Gamma_n(T, \varepsilon) = \{\lambda \in \Omega: \gamma_n(\lambda) < \varepsilon\}$, then (in the Attouch-Wets metric) $\lim_{n \to \infty} \Gamma_n(T, \varepsilon) = \operatorname{Sp}_{\varepsilon}(T), \qquad \Gamma_n(T, \varepsilon) \subset \operatorname{Sp}_{\varepsilon}(T).$

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

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

 $R = 5772.22, \omega = 0.264002$
 $A(\lambda)\phi = \left[\frac{1}{R}B(\lambda)^2 + i(\lambda U(y) - \omega)B(\lambda) + i\lambda U''(y)\right]\phi$
 $B(\lambda)\phi = -\frac{d^2\phi}{dy^2} + \lambda^2\phi, \ \langle \phi, \psi \rangle = \int_{-1}^{1} \phi \bar{\psi} + \frac{d\phi}{dy} \frac{d\psi}{dy} dy, \ T(\lambda) = B(\lambda)^{-1}A(\lambda)$

v

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

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

$$R = 5772.22, \omega = 0.264002$$

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







Which do we trust?





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

Computational tool #2: Contour methods

KELDYSH's THEOREM: Suppose $Sp_{ess}(T) \cap \Omega = \emptyset$. Then for $z \in \Omega \setminus Sp(T)$ $T(z)^{-1} = V(z - I)^{-1}W^* + R(z)$

- 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.

 \Rightarrow 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 Sp(*T*)).

$$A_0 = \frac{1}{2\pi i} \int_{\Gamma} T(z)^{-1} \mathcal{V} dz, \qquad A_1 = \frac{1}{2\pi i} \int_{\Gamma} zT(z)^{-1} \mathcal{V} dz \qquad \text{Random vectors} \\ \text{Gaussian process}$$

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 $\approx \mathcal{U}\Sigma_0 x_j$

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:
$$m = \text{Trace}\left(\frac{1}{2\pi i}\int_{\Gamma} T'(z)T(z)^{-1} dz\right)$$
 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.

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

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 $||\tilde{A}_j - A_j|| \le \varepsilon$.

THEOREM: For sufficiently oversampled \mathcal{V} , with overwhelming probability, $|\sigma_{\inf}(F(z)) - \sigma_{\inf}(\tilde{F}(z))| \le 2(\varepsilon + ||VJW^*||\varepsilon/\sigma_m(VW^*) + |z|\varepsilon)$ (quad. err.) $\operatorname{Sp}_{\underline{\|VW^*\|\|VW^*V\|+M\varepsilon}}(T) \subset \operatorname{Sp}_{\varepsilon}(F) \subset \operatorname{Sp}_{\underline{\sigma_m(VW^*)\sigma_m(VW^{*\mathcal{V}})-M\varepsilon}}(T).$ \Rightarrow converges **NOT** a statement on computing $Sp_{\varepsilon}(T)$ no spectral pollution (the other algorithm does that!) no spectral invisibility method is stable • C., Townsend, "Avoiding discretization issues for nonlinear eigenvalue problem", preprint. Stability bound

- Horning, Townsend, "FEAST for differential eigenvalue problems," SIAM J. Math. Anal., 2020.
- C., "Computing semigroups with error control," SIAM J. Math. Anal., 2022.

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

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

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

$$F(z)L_{2}[T(z)^{-1} - R(z)] = -VW^{*}$$
$$\|T(z)^{-1}\| > \varepsilon \Longrightarrow \sigma_{\inf}(F(z)) < \frac{\|VW^{*}\|\|VW^{*}\mathcal{V}\|}{1 - M\varepsilon}\varepsilon$$

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

Discretized using FEM (n =discretization size)

Example 1: One-dimensional acoustic wave



Example 1: One-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 2: Butterfly

Discretized $\mathcal{P}_n T(\lambda) \mathcal{P}_n^*$ (n = 500) Method based on γ_n 3 3 1e-02 1e-02 2 2 1e-04 1e-04 1e-06 1e-06 $\operatorname{Im}(\lambda)$ $\operatorname{Im}(\lambda)$ 1e-08 1e-08 0 1e-10 1e-10 -1 -1 1e-12 1e-12 -2 -2 1e-14 1e-14 -3 1e-16 -3 1e-16 -2 -3 -2 -1 2 3 -3 2 3 0 -1 0 1 $\operatorname{Re}(\lambda)$ $\operatorname{Re}(\lambda)$

Example 3: Loaded string

damped_beam from NLEVP collection.



planar_waveguide from NLEVP collection.

$$\frac{\mathrm{d}^2 \phi}{\mathrm{d}x^2} + k^2 \left(\eta^2 - \mu(\lambda)\right) \phi = 0$$
$$\mu(\lambda) = \frac{\delta_+}{k^2} + \frac{\delta_-}{8k^2\lambda^2} + \frac{\lambda^2}{k^2}$$
$$\frac{\mathrm{d}\phi}{\mathrm{d}x}(0) + \left(\frac{\delta_-}{2\lambda} - \lambda\right) \phi(0) = 0$$
$$\frac{\mathrm{d}\phi}{\mathrm{d}x}(2) + \left(\frac{\delta_-}{2\lambda} + \lambda\right) \phi(2) = 0$$

 η corresponds to refractive index.

 λ correspond to guided and leaky modes. Discretized using FEM (n = 129, default)







12/14



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 $\sigma_{\inf}(T)$, e.g., compute $\sigma_{\inf}(T\mathcal{P}_n^*)$ or $\sqrt{\sigma_{\inf}(\mathcal{P}_nT^*T\mathcal{P}_n^*)}$
 - 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 $(A zI)^{-1}$ or $T(z)^{-1}$
 - 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.
- InfBeyn overcomes these in regions of discrete spectra: convergent, stable, efficient.
- Compute pseudospectra (of generic pencils) with explicit error control

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 problem", 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."