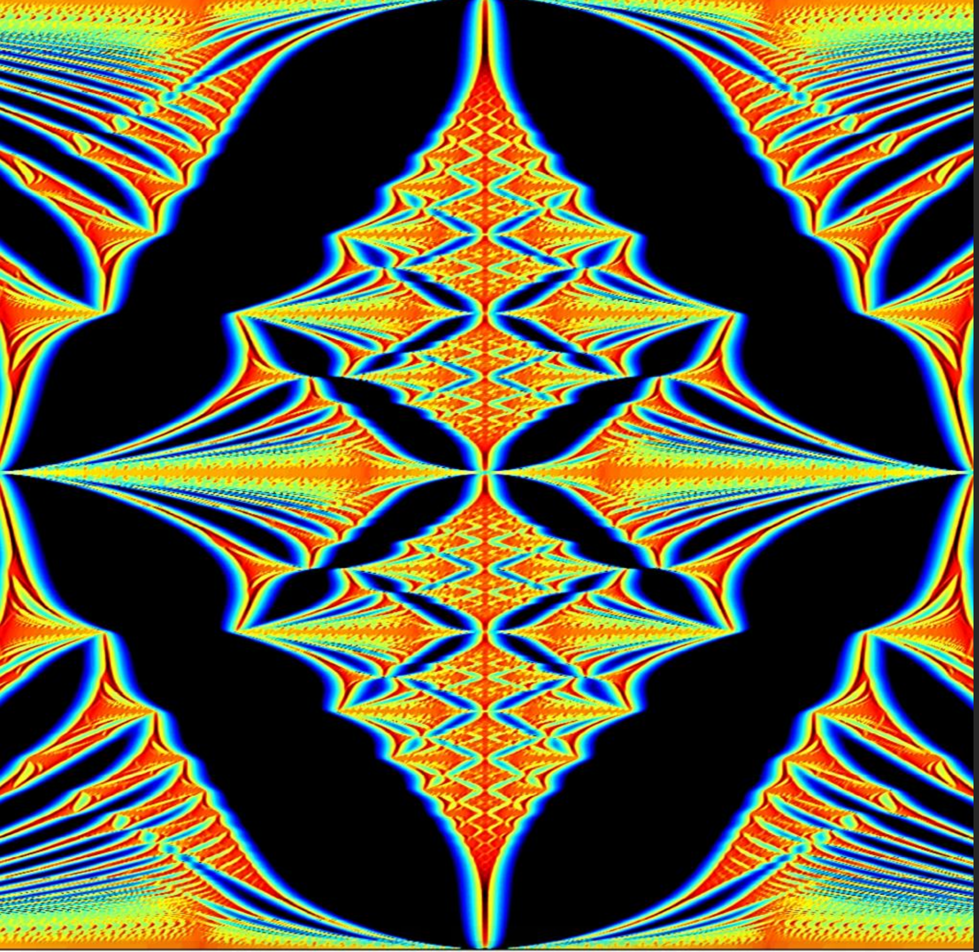

Spectral Computations in Infinite Dimensions

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Left to right: Vegard Antun (Oslo), Lorna Ayton (Cambridge), Jonathan Ben-Artzi (Cardiff), Anders Hansen (Cambridge), Andrew Horning (MIT), Olavi Nevanlinna (Aalto), Bogdan Roman (Cambridge), Markus Seidel (West Saxon), Matt Szőke (Virginia Tech), Kyle Thicke (Texas A&M), Alex Townsend (Cornell), Alex Watson (Minnesota)

Linear spectral problem

$$A \text{"="} \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \qquad A\left(\sum_{k=1}^{\infty} x_k e_k\right) = \sum_{j=1}^{\infty}\left(\sum_{k=1}^{\infty} a_{jk} x_k\right) e_j$$

Canonical basis vectors of $l^2(\mathbb{N})$

Finite-dimensional	$\Longrightarrow$	Infinite-dimensional
Eigenvalues of $B \in \mathbb{C}^{n\times n}$	$\Longrightarrow$	Spectrum, $\mathrm{Sp}(A)$
$\{\lambda_j \in \mathbb{C}: \det(B - \lambda_j I) = 0\}$	$\Longrightarrow$	$\{\lambda \in \mathbb{C}: A - \lambda I \text{ is not invertible}\}$

*"Most operators that arise in practice are not presented in a representation in which they are diagonalized, and it is often very hard to locate even a single point in the spectrum. Thus, one often has to settle for numerical approximations [...] Unfortunately, there is a dearth of literature on this basic problem and, so far as we have been able to tell, **there are no proven [general] techniques**."* W. Arveson, Berkeley (1994)

A motivating problem

In a series of papers in the 1950's and 1960's, J. Schwinger examined the foundations of quantum mechanics. A key problem he considered:

Given a self-adjoint Schrödinger operator $-\Delta + V$ on $\mathbb{R}$, can we approximate its spectrum?

Partial answer: T. Digernes, V. S. Varadarajan and S. R. S. Varadhan (1994) gave a convergent algorithm for a class of V generating compact resolvent.

For which classes of differential operators on unbounded domains do there exist algorithms that converge to the spectrum? Can we guarantee that the output is in the spectrum up to an arbitrarily small tolerance?

- Digernes, Varadarajan, Varadhan, "*Finite approximations to quantum systems*," **Rev. Math. Phys.**, 1994.

What can go wrong?

Matrix case ($l^2(\mathbb{N})$): truncate to $\mathcal{P}_n A \mathcal{P}_n^* \in \mathbb{C}^{n\times n}$.

PDE on unbounded domain: truncate domain then discretise.

Some key issues:

- Spectral pollution (evals accumulate at pts not in $\mathrm{Sp}(A)$ as $n \to \infty$)
- Spectral invisibility.
- Dealing with essential spectra and continuous spectra.
- Stability, non-normality etc.
- Verification – can we compute spectral properties with error bounds?

- Boegli, Marletta, Tretter, *The essential numerical range for unbounded linear operators,"* **J. Funct. Anal.**, 2020.

Not all spectral problems are created equal …

Warm-up: bounded diagonal operators

$$A = \begin{pmatrix} a_1 & & \\ & a_2 & \\ & & \ddots \end{pmatrix}$$

Assumption: Algorithm can query entries of A

Algorithm: $\Gamma_n(A) = \{a_1, a_2, \ldots, a_n\} \to \mathrm{Sp}(A) = \overline{\{a_1, a_2, \ldots\}}$ in Haus. Metric.

One-sided error control: $\Gamma_n(A) \subset \mathrm{Sp}(A)$

$$d_{\mathrm{H}}(X, Y) = \max\left\{\sup_{x \in X} d(x, Y), \sup_{y \in Y} d(y, X)\right\}$$

Optimal: Can't obtain $\hat{\Gamma}_n(A) \to \mathrm{Sp}(A)$ with $\mathrm{Sp}(A) \subset \hat{\Gamma}_n(A)$.

Example: compact self-adjoint operators

classic method

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Algorithm: $\Gamma_n(A) = \mathrm{Sp}(\mathcal{P}_n A \mathcal{P}_n^*)$ converges to $\mathrm{Sp}(A)$ in Haus. Metric.

Question: Can we verify the output?

i.e., Does there exist some alg. $\widehat{\Gamma}_n(A) \to \mathrm{Sp}(A)$ with $\widehat{\Gamma}_n(A) \subset \mathrm{Sp}(A) + B_{2^{-n}}$?

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Answer: No algorithm can do this on whole class!

What about Jacobi operators?

$$A = \begin{pmatrix} a_1 & b_1 & & \\ b_1 & a_2 & b_2 & \\ & b_2 & a_3 & \ddots \\ & & \ddots & \ddots \end{pmatrix}, \qquad b_k > 0, \qquad a_k \in \mathbb{R}$$

Non-trivial, e.g., spurious eigenvalues.

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Non-trivial, e.g., spurious eigenvalues.

Enlarge class to **sparse normal operators** - surely now much harder?!

Answer: $\exists\{\Gamma_n\}$ s.t. $\lim_{n\to\infty} \Gamma_n(A) = \mathrm{Sp}(A)$ and $\Gamma_n(A) \subset \mathrm{Sp}(A) + B_{2^{-n}}$,

for any sparse normal operator A

- C., Roman, Hansen, "How to compute spectra with error control," **Phys. Rev. Lett.**,,2019.

General bounded:

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Hansen's three-limit algorithm

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

- Hansen, *"On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators,"* **J. Am. Math. Soc.**, 2011.

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$$n_2 \rightarrow \qquad n_1 \downarrow \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

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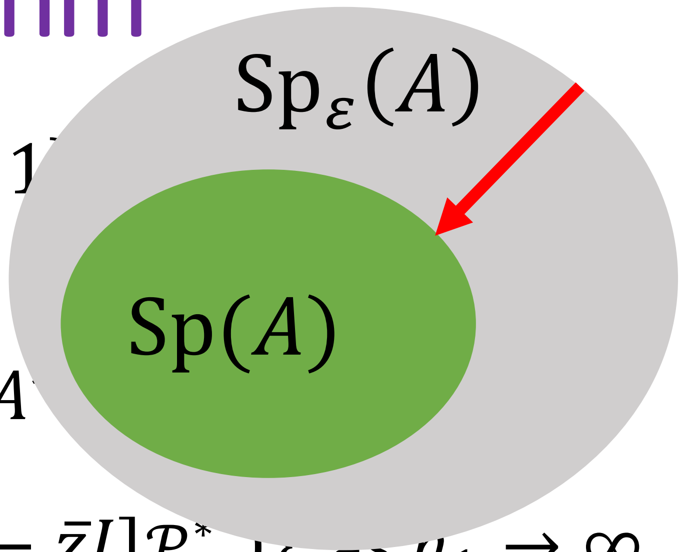

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Approx. pseudospectrum: $\lim_{n_2\to\infty} \lim_{n_1\to\infty} \hat{\Gamma}_{n_1,n_2}(A,\varepsilon) = \mathrm{Sp}_\varepsilon(A) = \{z : \gamma(A,z) \le \varepsilon\}$

$$\Gamma_{n_1,n_2,n_3}(A) = \hat{\Gamma}_{n_1,n_2}(A, 1/n_3)$$

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$\sigma_{\inf}(A) = \inf\{\| \ldots (A) \| \ldots$

$\gamma_{n} \ldots \inf\{\sigma_{\inf}(\ldots zI]\mathcal{P}_{n_2}^{*})\}$

$\gamma_{n_1,n_2}(A,z) \ldots \gamma_{n_2}(A \ldots \sigma_{\inf}([A^* - \bar{z}I]\mathcal{P}_{n_2}^{*})\}$, as $n_1 \to \infty$

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Can show three limits is sharp!

Embed canonical problems such as:

Given $B \in \{0,1\}^{\mathbb{N}\times\mathbb{N}}$, does B have a col. with inf. many 1's?

$\Longrightarrow$ lower bounds (indep. of comp. model).

- Hansen, *"On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators,"* **J. Am. Math. Soc.**, 2011.
- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, *"On the solvability complexity index hierarchy and towers of algorithms,"* preprint.
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Hansen's three-limit algorithm

Can show three limits is sharp!

Explains Arveson's lament!

$$\sigma_{\mathrm{inf}}(A) = \mathrm{inf}\{\| \ldots (A), \|v\| = \ldots\}$$

$$\gamma_{n} \ldots \mathrm{in}\{\sigma_{\mathrm{inf}}(\mathcal{P}_{n} [A \ldots]), \sigma_{\mathrm{inf}}(\mathcal{P}_{n_1}[A^* - \bar{z}I]\mathcal{P}_{n_2}^*)\}$$

$$\gamma_{n_1,n_2}(A,z) \downarrow \gamma_{n_2}(A,z) \ldots ([A - zI]\mathcal{P}_{n_2}^*), \sigma_{\mathrm{inf}}([A^* - \bar{z}I]\mathcal{P}_{n_2}^*)\}, \text{ as } n_1 \to \infty$$

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WHAT ASSUMPTIONS ARE NEEDED TO GET PAST THIS?

$\sigma_{\inf}(A) = \inf\{\| \ldots (A), \|v\| \ldots \}$

$\gamma_{n} \ldots \{\sigma_{\inf}(\mathcal{P}_{n} [A \ldots]), \sigma_{\inf}(\mathcal{P}_{n_1}[A^* \ldots \}$

$\gamma_{n_1,n_2}(A, z) \ldots \gamma_{n_2}(A, z) \ldots ([A - zI]\mathcal{P}^*_{\ldots}) \ldots zI]\mathcal{P}^*_{n_2})\}$, as $n_1 \to \infty$

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Solvability Complexity Index Hierarchy

Class $\Omega \ni A$, want to compute $\Xi\colon \Omega \to (\mathcal{M}, d)$ ← metric space

- Δ_0: Problems solved in finite time (v. rare for cts problems).
- Δ_1: Problems solved in "one limit" with full error control:

$$d(\Gamma_n(A), \Xi(A)) \le 2^{-n}$$

- Δ_2: Problems solved in "one limit":

$$\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$$

- Δ_3: Problems solved in "two successive limits":

$$\lim_{n\to\infty} \lim_{m\to\infty} \Gamma_{n,m}(A) = \Xi(A)$$

⋮

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⋮

Can work in *any* computational model. BUT in infinite dimensions, spectral problems are just as hard from a foundations point of view if we use a BSS machine, Turing machine, interval arithmetic etc.

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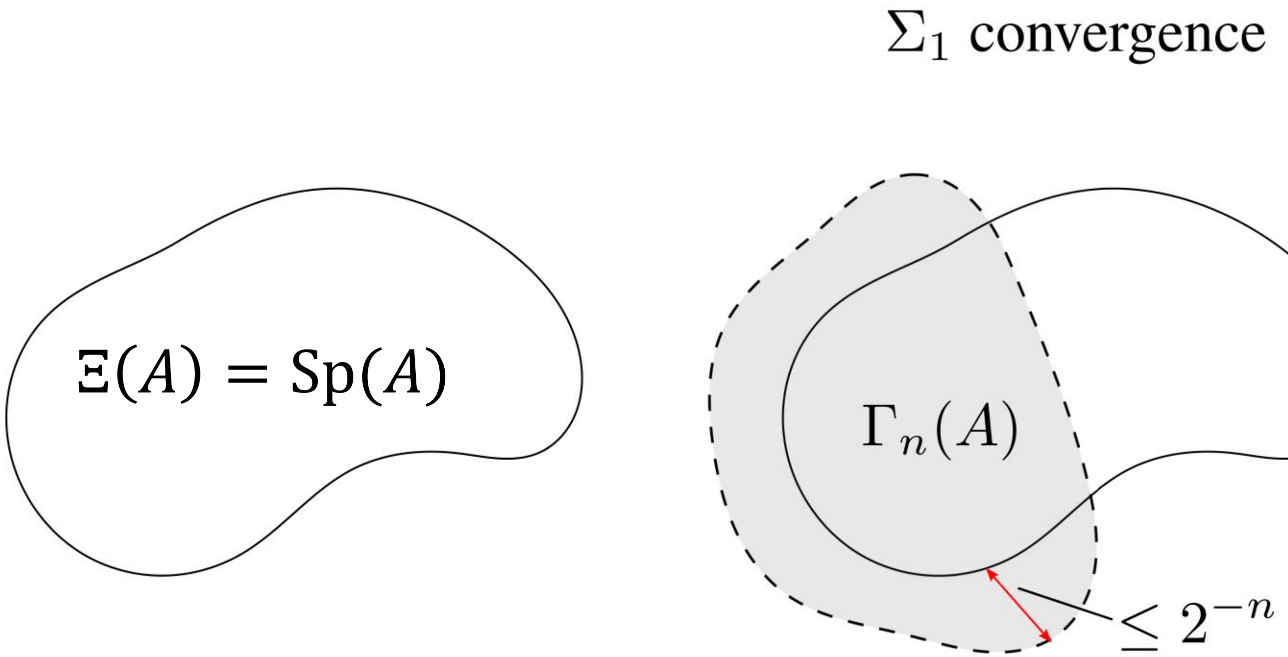
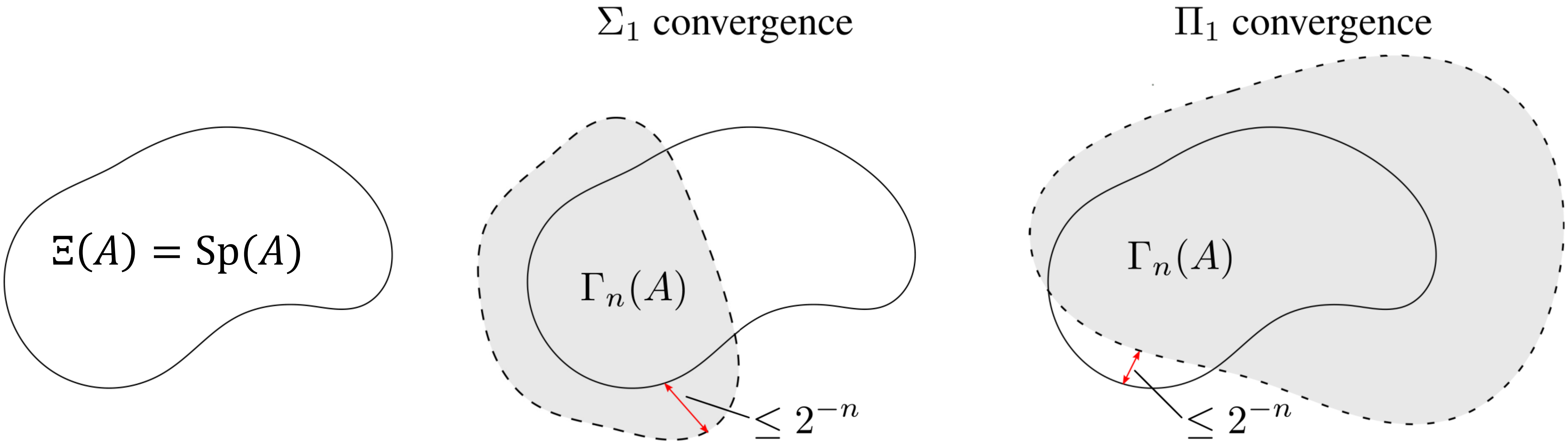
Error control for spectral problems



- Σ_1: $\exists$ alg. $\{\Gamma_n\}$ s.t. $\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$, $\max_{z\in\Gamma_n(A)} \mathrm{dist}\big(z, \Xi(A)\big) \leq 2^{-n}$

Error control for spectral problems



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- Π_1: $\exists$ alg. $\{\Gamma_n\}$ s.t. $\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$, $\max_{z\in\Xi(A)} \mathrm{dist}(z, \Gamma_n(A)) \leq 2^{-n}$

Such problems can be used in a proof!

Sample: some results for bounded op. on $l^2(\mathbb{N})$

increasing difficulty →

Error control | **1 limit** | **2 limits** | **3 limits**

$$\Pi_0 = \Delta_0 = \Sigma_0 \subsetneq \Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \cdots$$

$$\Delta_1 \subsetneq \Pi_1 \subsetneq \Delta_2, \quad \Delta_1 \subsetneq \Sigma_1 \subsetneq \Delta_2$$

$$\Delta_2 \subsetneq \Pi_2 \subsetneq \Delta_3, \quad \Delta_2 \subsetneq \Sigma_2 \subsetneq \Delta_3$$

$$\Delta_3 \subsetneq \Pi_3 \cdots, \quad \Delta_3 \subsetneq \Sigma_3 \cdots$$

Sample: some results for bounded op. on $l^2(\mathbb{N})$

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Compact operators → Δ_2

$$\Pi_0 = \Delta_0 = \Sigma_0$$

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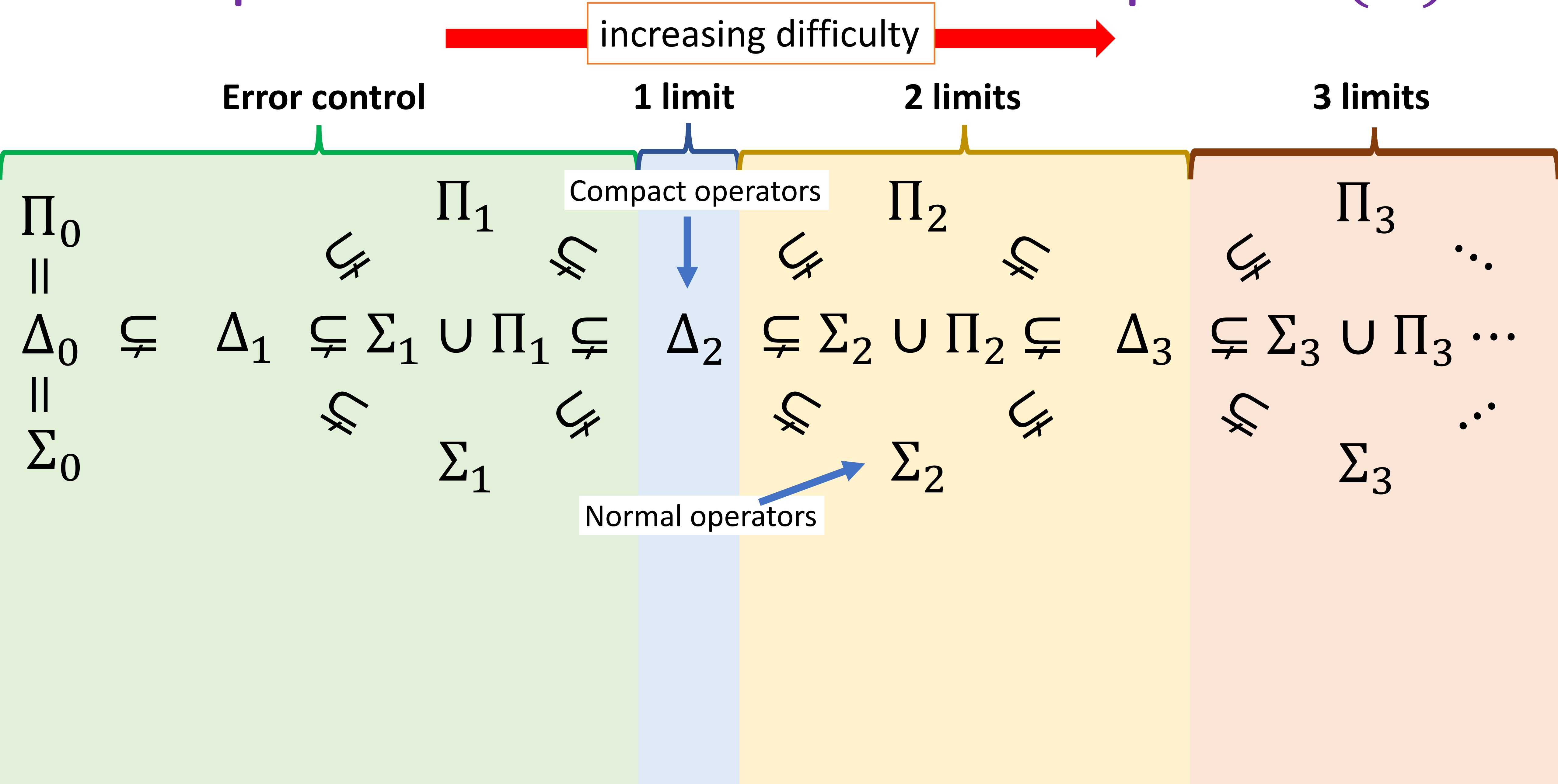

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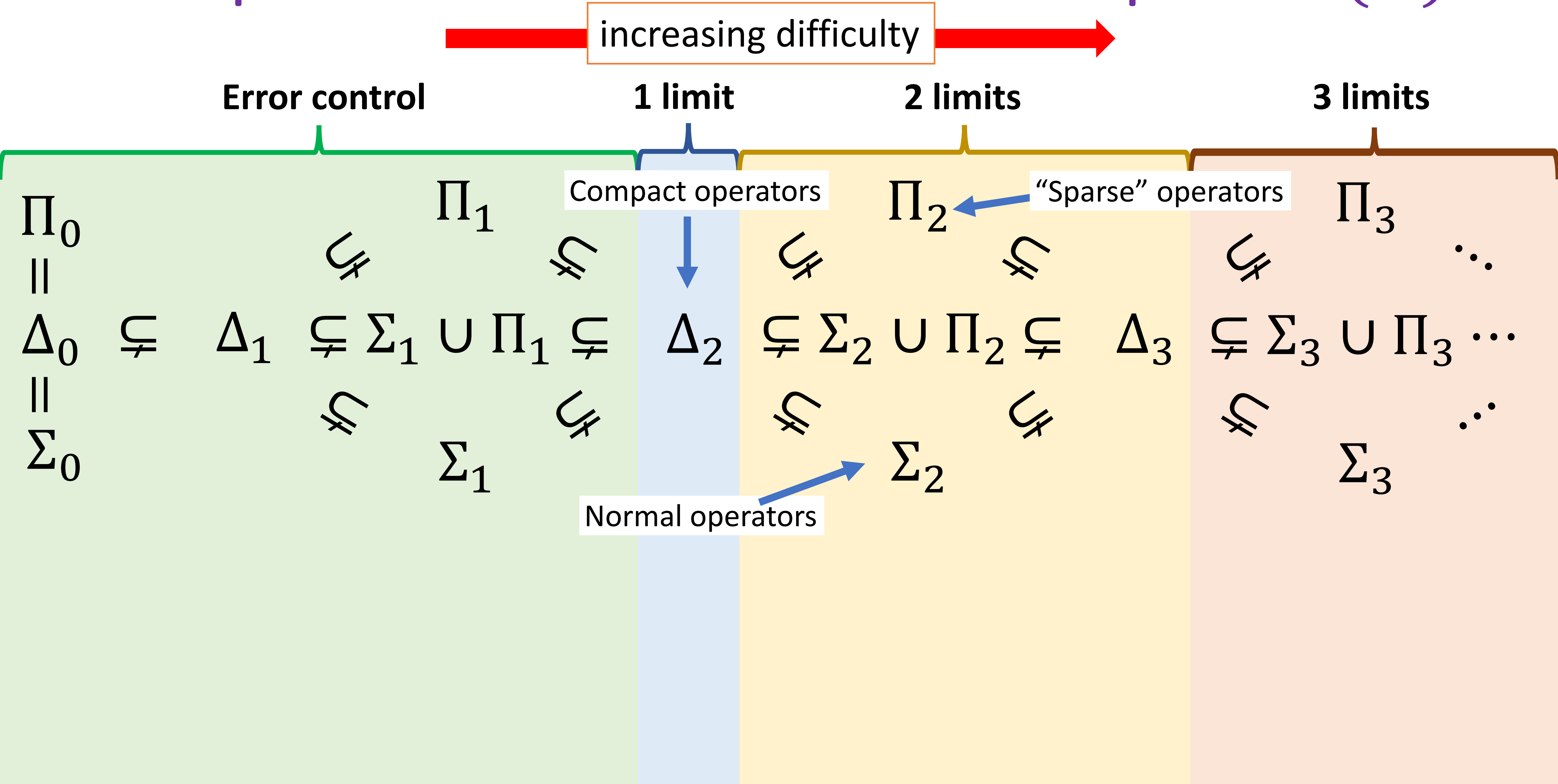

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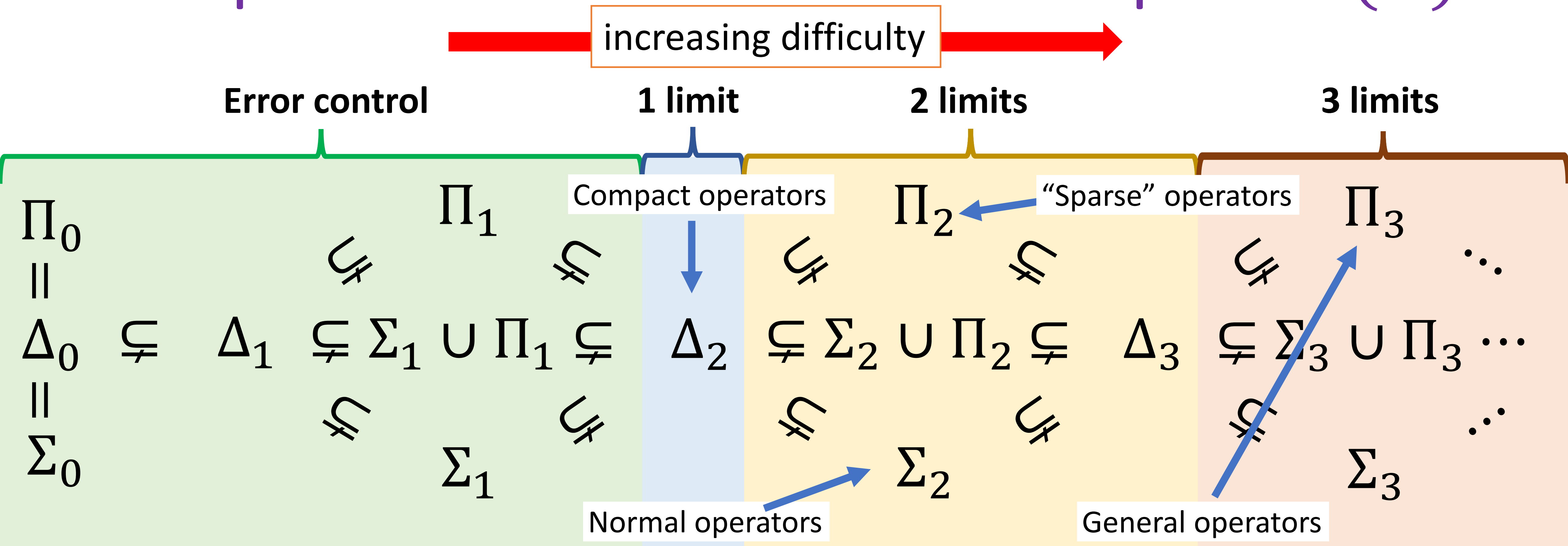

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Π_0 Π_1 Π_2 Π_3

$$\Pi_0 = \Delta_0 = \Sigma_0$$

$$\Delta_0 \subsetneq \Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \cdots$$

Σ_0 Σ_1 Σ_2 Σ_3

Compact operators → Δ_2

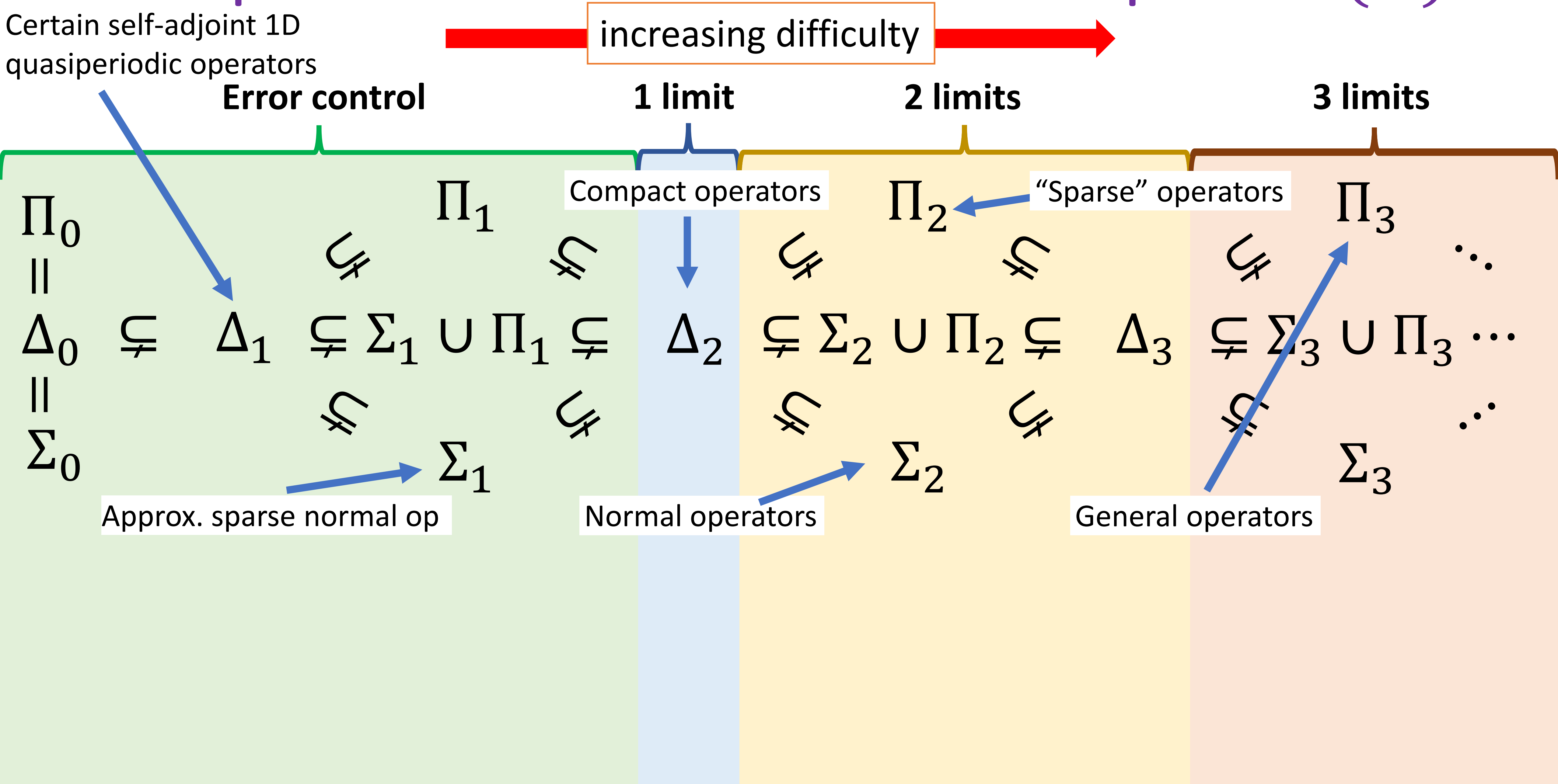
"Sparse" operators → Π_2

Approx. sparse normal op → Σ_1

Normal operators → Σ_2

General operators → Π_3

Sample: some results for bounded op. on $l^2(\mathbb{N})$



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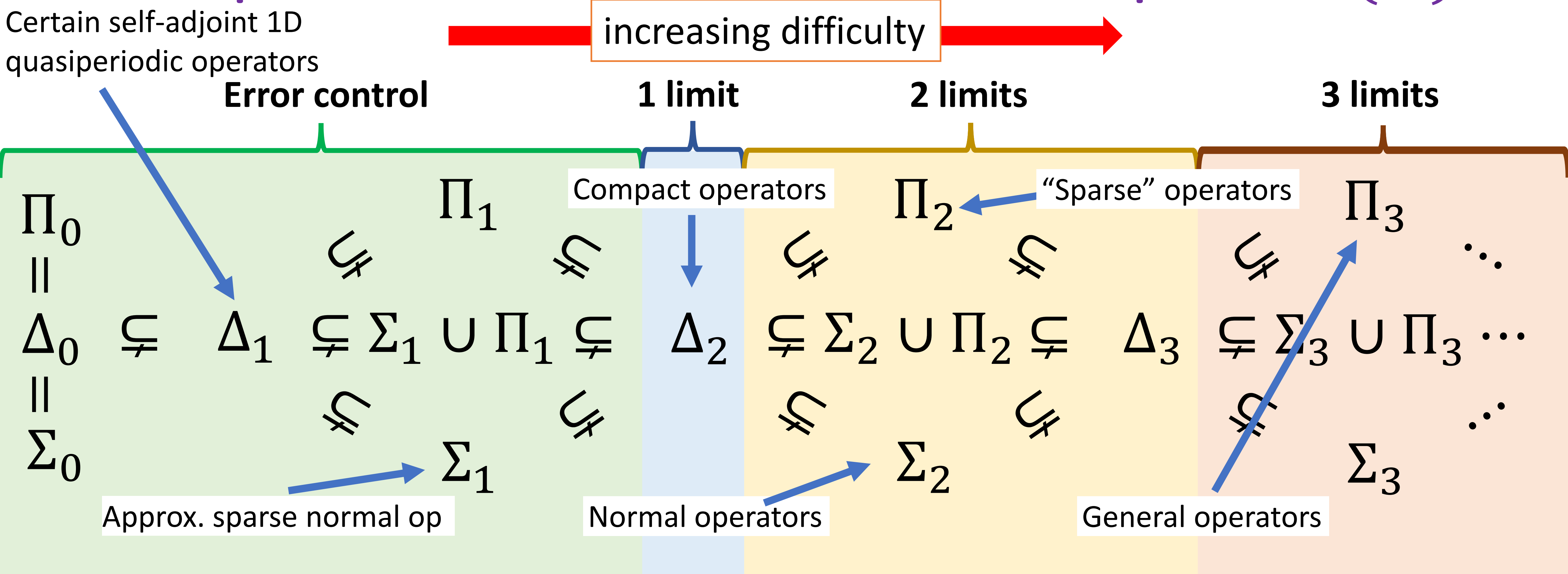

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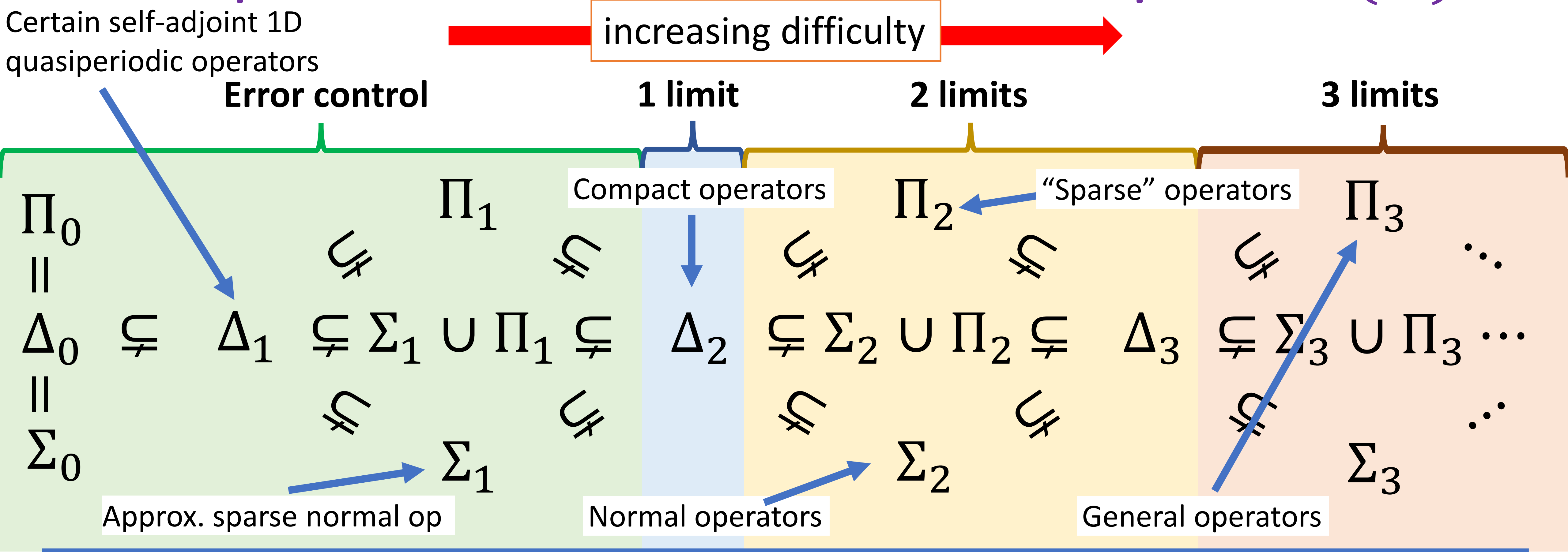
Zoo of problems: spectral type (pure point, absolutely continuous, singularly continuous), Lebesgue measure and fractal dimensions of spectra, discrete spectra, essential spectra, eigenspaces + multiplicity, spectral radii, essential numerical ranges, geometric features of spectrum (e.g., capacity), spectral gap problem, resonances ...

Sample: some results for bounded op. on $l^2(\mathbb{N})$



- 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.

Back to Schwinger: $-\Delta + V$ on $L^2(\mathbb{R}^d)$

Theorem: Let Ω be class of self-adjoint diff. operators on $L^2(\mathbb{R}^d)$ of the form

$$T = \sum_{k\in\mathbb{Z}^d_{\geq 0},|k|\leq N} c_k(x)\,\partial^k \qquad \text{s.t.}$$

- Smooth compactly supported functions form a core of T.
- $\{c_k\}$ are polynomially bounded and of locally bounded total variation.

Assume algorithm can:

- Point sample $\{c_k(q)\}$ for $q\in\mathbb{Q}^d$ to arbitrary prec.
- Evaluate a polynomial that bounds $\{c_k\}$ on $\mathbb{R}^d$.

Then…

- C., Hansen, *"The foundations of spectral computations via the solvability complexity index hierarchy,"* **J. Eur. Math. Soc.**, 2022

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Then

Verifiable

Not verifiable

(a) Know bound $\mathrm{TV}_{[-n,n]^d}(c_k) \leq b_n \Longrightarrow \{\mathrm{Sp}, \Omega\} \in \Sigma_1$.

(b) Only know asymp. bound $\mathrm{TV}_{[-n,n]^d}(c_k) = O(b_n) \Longrightarrow \{\mathrm{Sp}, \Omega\} \in \Delta_2 \backslash (\Sigma_1 \cup \Pi_1)$.

- C., Hansen, *"The foundations of spectral computations via the solvability complexity index hierarchy,"* **J. Eur. Math. Soc.**, 2022

Back to Schwinger: $-\Delta + V$ on $L^2(\mathbb{R}^d)$

increasing difficulty →

Error control | **1 limit** | **2 limits** | **3 limits**

Can "nearly" do it for imaginary cubic oscillator! (→ Δ_1)

Unbounded, sectorial V (→ Δ_2)

Bounded V with locally bounded TV (→ Π_2)

Bounded V (→ Π_3)

$$\Pi_0 = \Delta_0 = \Sigma_0$$

$$\Delta_0 \subsetneq \Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \cdots$$

$$\Delta_1 \subsetneq \Pi_1 \subsetneq \Delta_2, \quad \Delta_1 \subsetneq \Sigma_1 \subsetneq \Delta_2$$

$$\Delta_2 \subsetneq \Pi_2 \subsetneq \Delta_3, \quad \Delta_2 \subsetneq \Sigma_2 \subsetneq \Delta_3$$

$$\Delta_3 \subsetneq \Pi_3 \cdots, \quad \Delta_3 \subsetneq \Sigma_3 \cdots$$

Self-adjoint, bounded V with locally bounded TV (→ Σ_1)

NB: Most existing convergence results for spectra, even on bounded domains, prove Δ_2 results and miss the optimal Σ_1 convergence!

CHALLENGE: Can you get Σ_1 for your problem/method?

Why study this hierarchy?

FOUNDATIONS $\longleftrightarrow$ NUMERICS

- $\mathrm{SCI} > 1$ classifications $\Longrightarrow$ tells us assumptions needed to lower SCI.
- Sharp classifications $\Longrightarrow$ new algorithms.
- Σ_1 and Π_1 classifications $\Longrightarrow$ look-up table for computer-assisted proofs.
- Negative results prevent us from trying to prove too much.
- Much of computational literature does not prove sharp results!

Remarks:

- Can use with any model of computation.
- Existing hierarchies (e.g., arithmetic, Baire etc.) included as particular cases.

Nonlinear spectral problems (NEPs)

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

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

$$\mathrm{Sp}(T) = \{\lambda \in \Omega: T(\lambda) \text{ is not invertible}\}$$
$$\mathrm{Sp_d}(T) = \{\lambda \in \mathrm{Sp}(T): T(\lambda) \text{ Fredholm}\}$$
$$\mathrm{Sp_{ess}}(T) = \mathrm{Sp}(T) \backslash \mathrm{Sp_d}(T)$$
$$\mathrm{Sp}_\varepsilon(T) = \mathrm{Closure}(\{\lambda \in \Omega: \|T(\lambda)^{-1}\| > 1/\varepsilon\})$$

Current known classifications:

- $\mathrm{Sp}_\varepsilon(A)$ is Σ_1 (sharp) for "generic" diff. operators, discrete operators etc.
- Hence spectrum is at worst Π_2.
- $\mathrm{Sp_d}(T)$ is Δ_2 (one limit, no error control) in regions with no ess. spec.

Keldysh's Theorem

Theorem: Suppose $\mathrm{Sp}_{\mathrm{ess}}(T) \cap \Omega = \emptyset$ and $\mathrm{Sp}(T) \neq \Omega$. Then for $z \in \Omega \backslash \mathrm{Sp}(T)$

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

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

Approximate these 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 $\|\tilde{A}_j - A_j\| \leq \varepsilon_j$ and let $\kappa = \frac{\|VW^*\|}{\sigma_m(VW^*)}$ (condition number).

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

$$\left|\sigma_{\inf}(F(z)) - \sigma_{\inf}(\tilde{F}(z))\right| \leq 2(\varepsilon_1 + \|VJW^*\|\varepsilon_0/\sigma_m(VW^*) + |z|\varepsilon_0) \text{ (quad. err.)}$$

Moreover, if $2M\kappa\varepsilon < 1$, then

$$\mathrm{Sp}_{\frac{\varepsilon}{\kappa}}(T) \subset \mathrm{Sp}_{\frac{2\|VW^*\|^2}{\kappa - M\varepsilon}\varepsilon}(F) \subset \mathrm{Sp}_{\frac{4\kappa\varepsilon}{1-2M\kappa\varepsilon}}(T).$$

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

$\Longrightarrow$ converges without spectral pollution or invisibility + method is stable.

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

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

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

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: two-dimensional acoustic wave

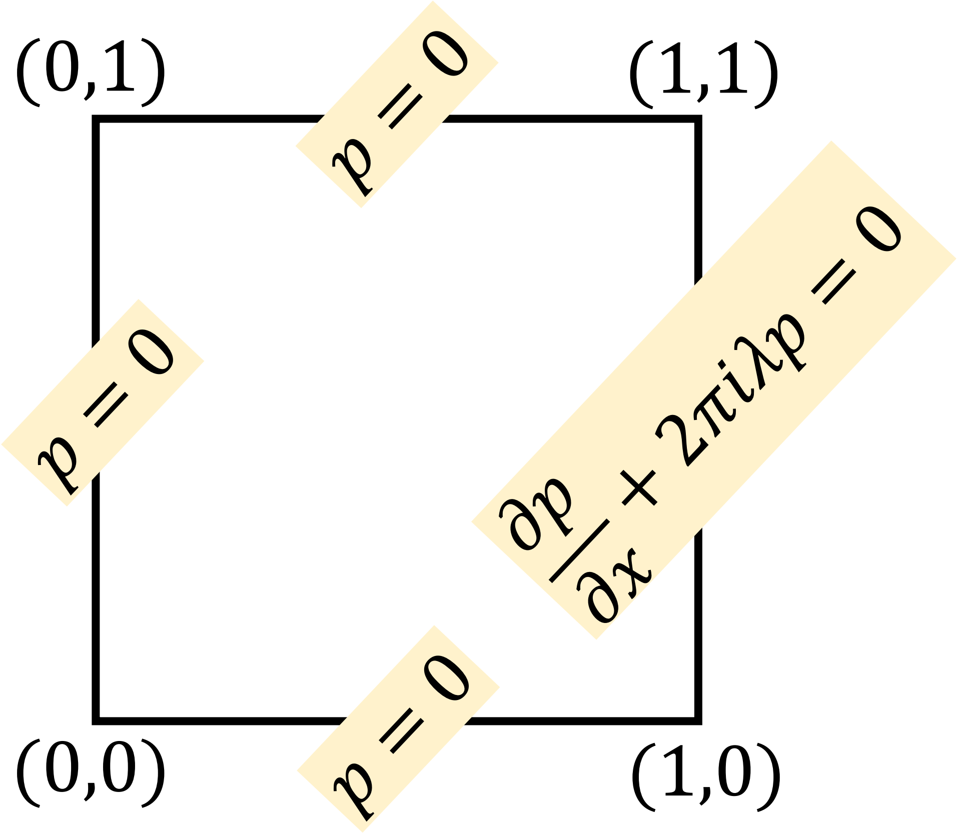
acoustic_wave_2d from NLEVP collection.

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

p corresponds to acoustic pressure.

λ correspond to resonant frequencies.

Discretised using FEM.



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

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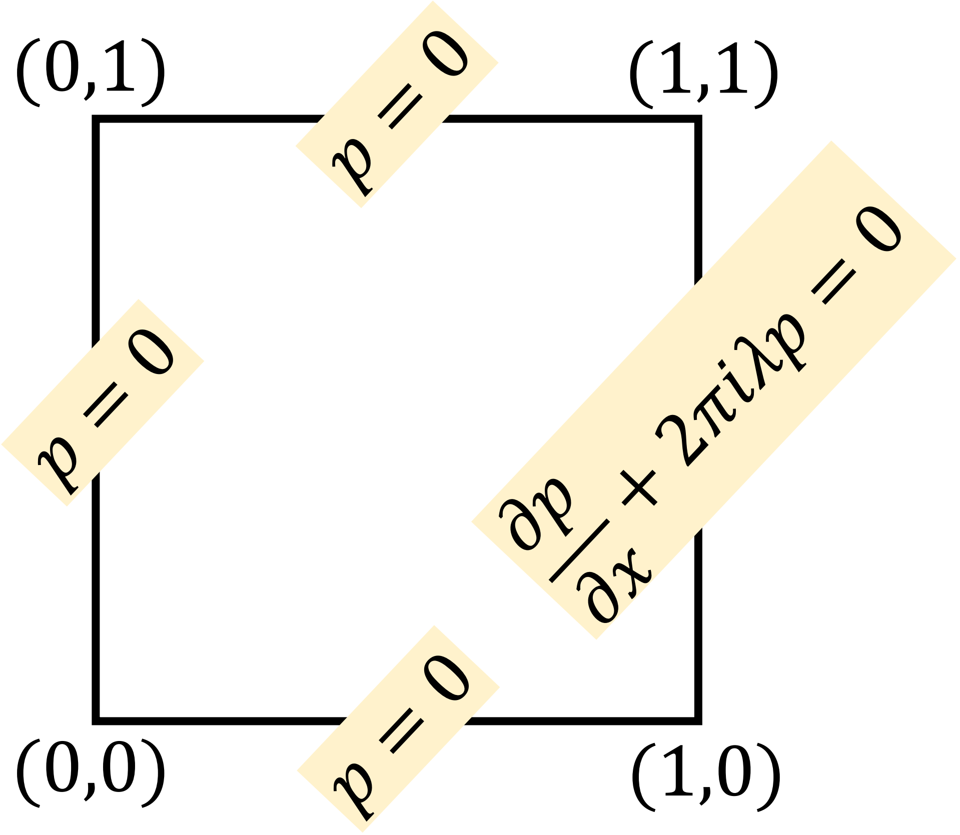
25 out of 52 come from an infinite-dimensional problem!



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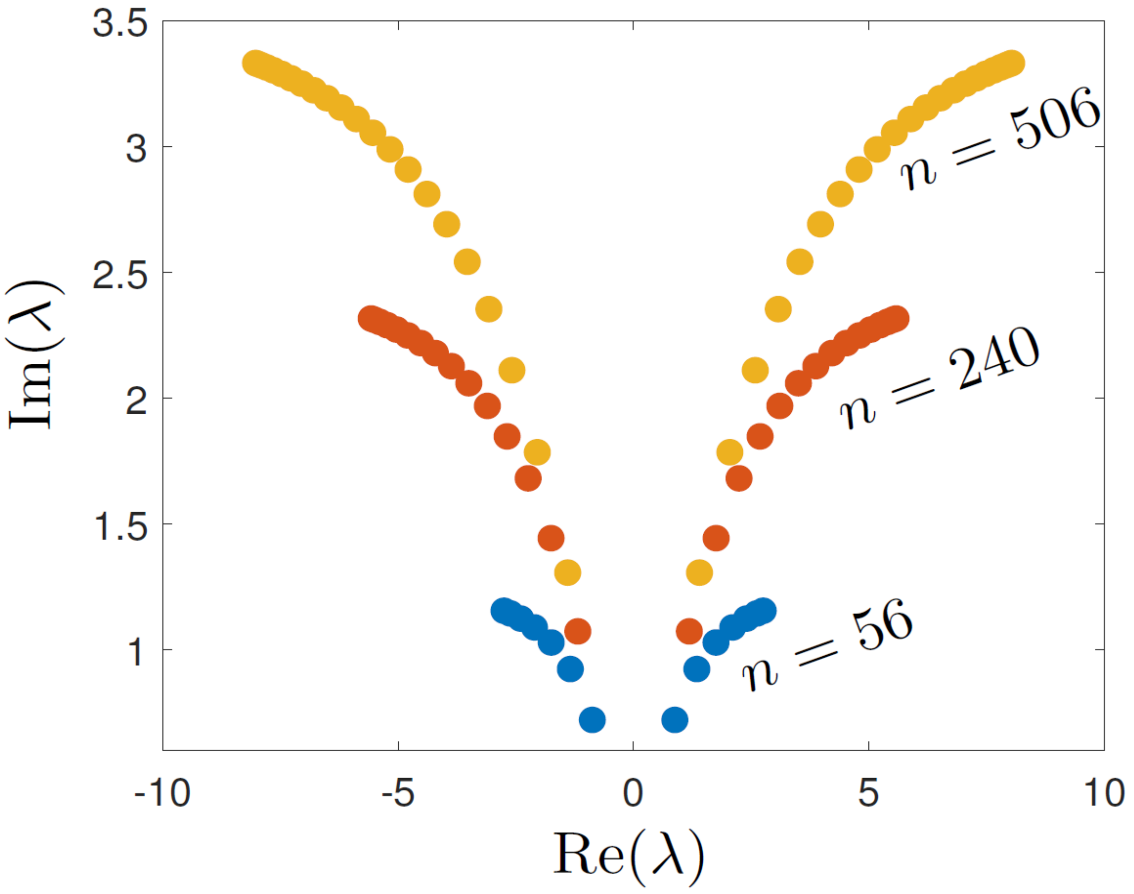
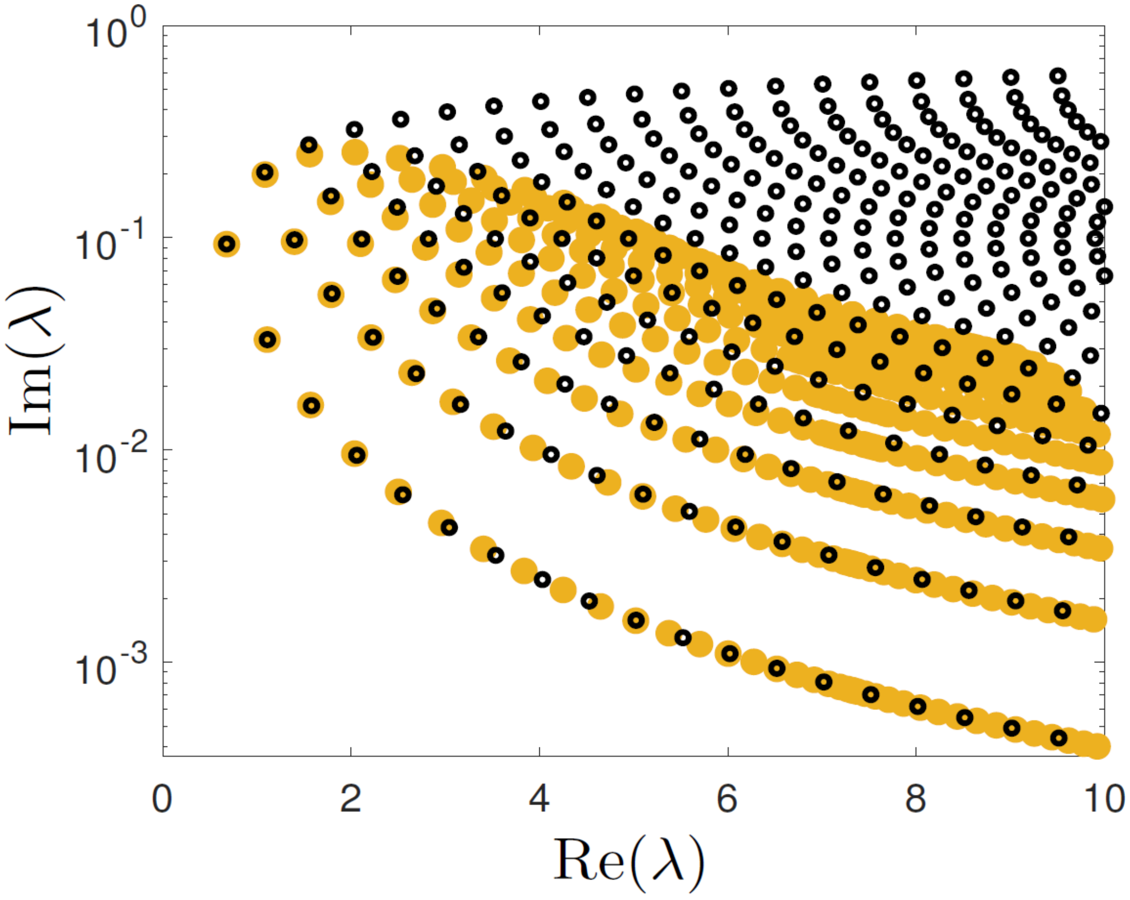


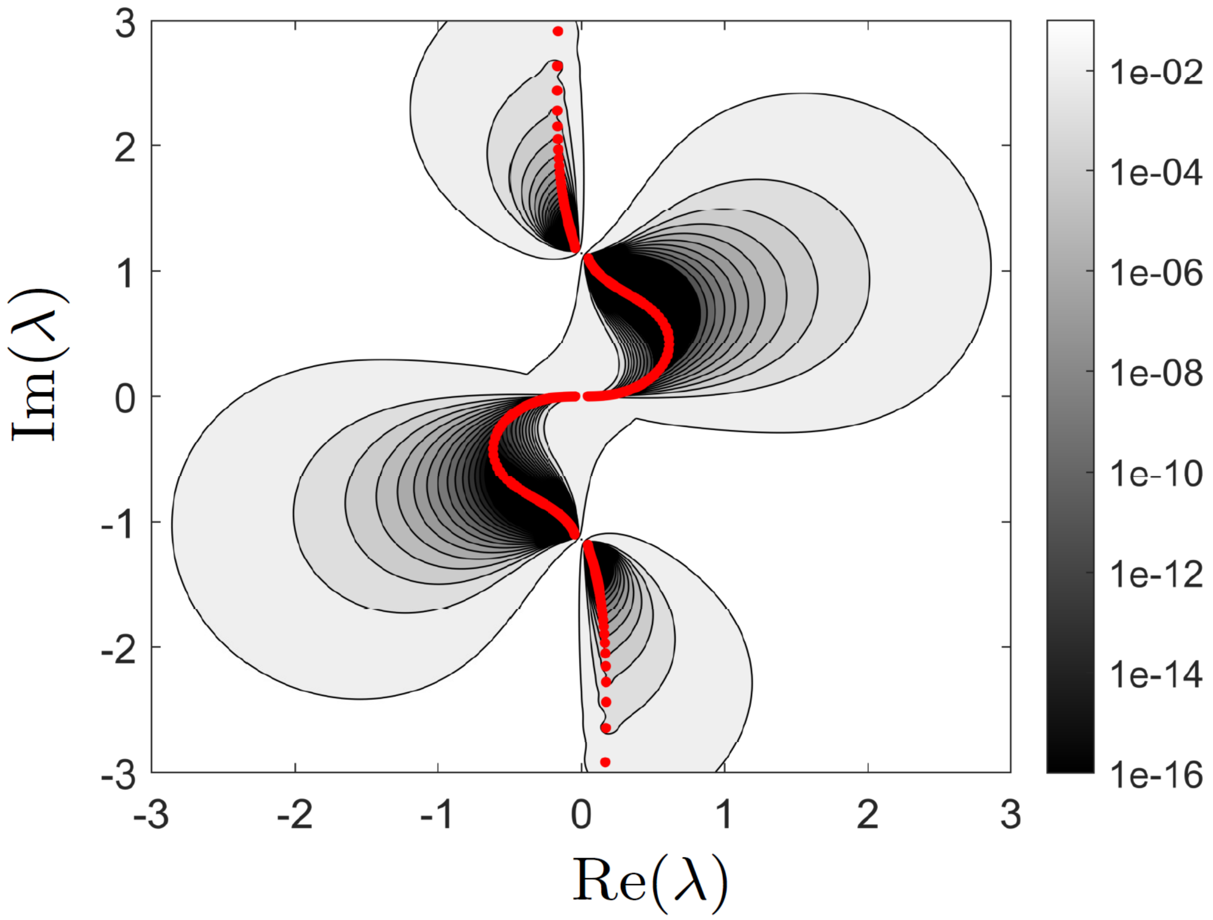


- C., Townsend, *"Avoiding discretization issues for nonlinear eigenvalue problem"*, preprint.

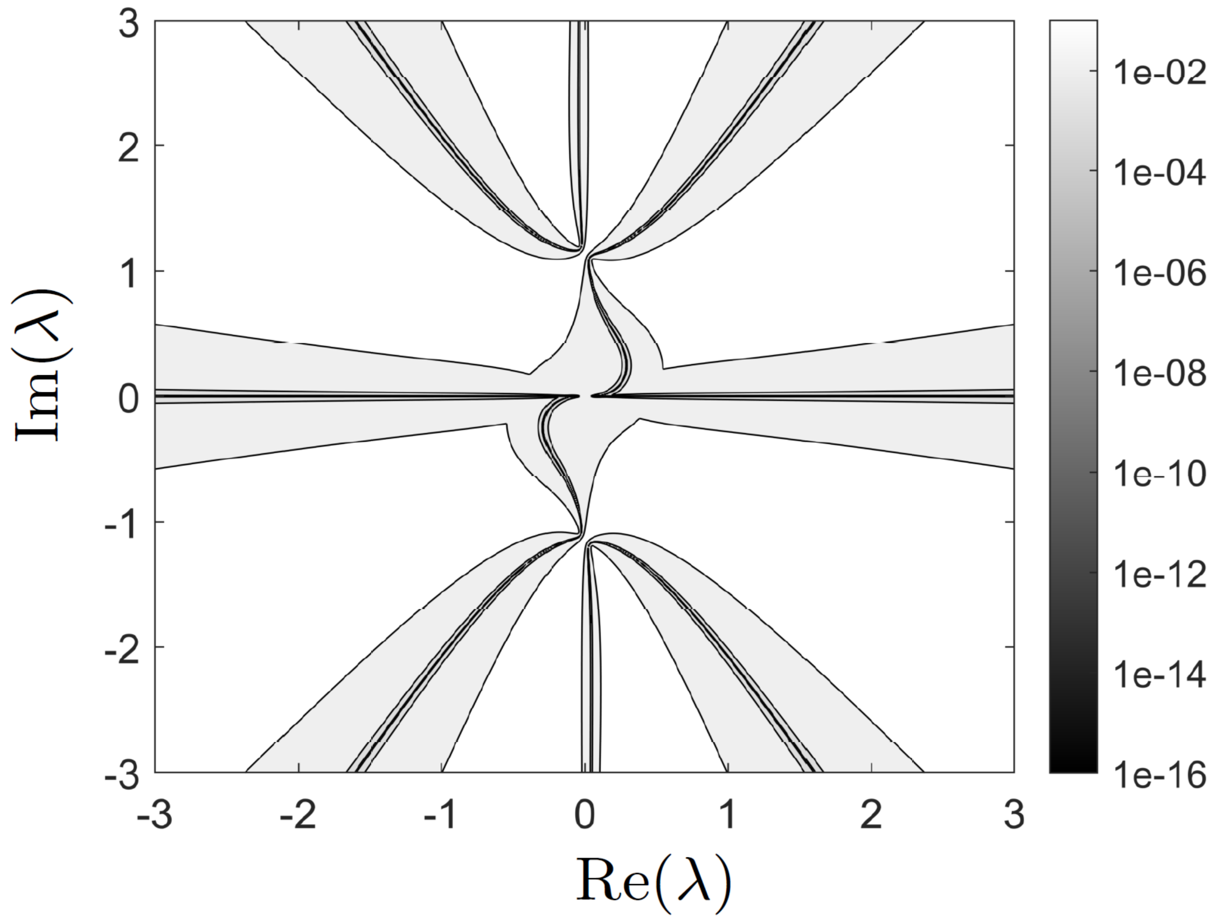
butterfly from NLEVP collection
$T(\lambda) = F(\lambda, S)$
S bilateral shift on $l^2(\mathbb{Z})$
F a rational function

Example: butterfly

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



Method based on $\sigma_{\text{inf}}(T(\lambda)\mathcal{P}_n^*)$



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

Example: planar waveguide

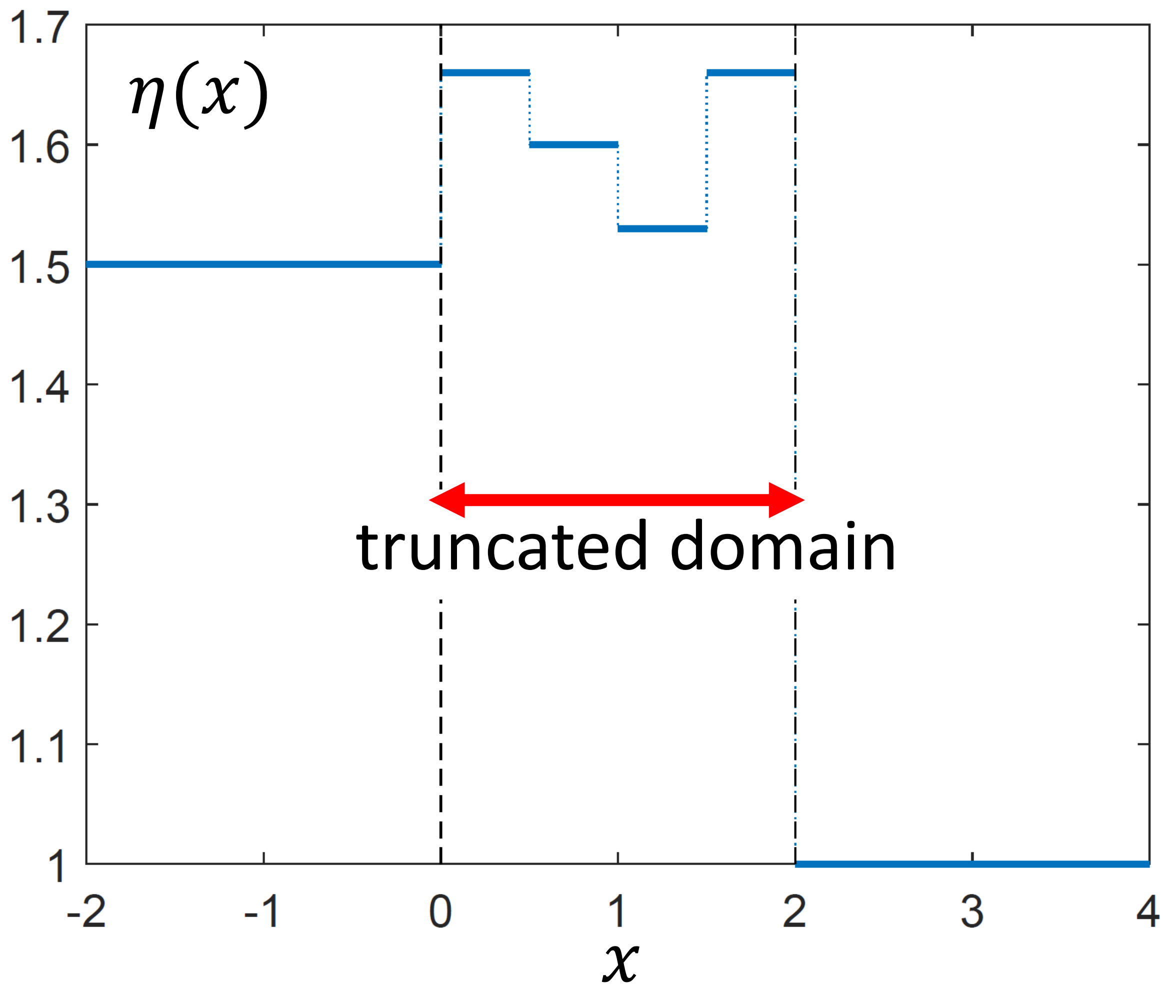
planar_waveguide from NLEVP collection.

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

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

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

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

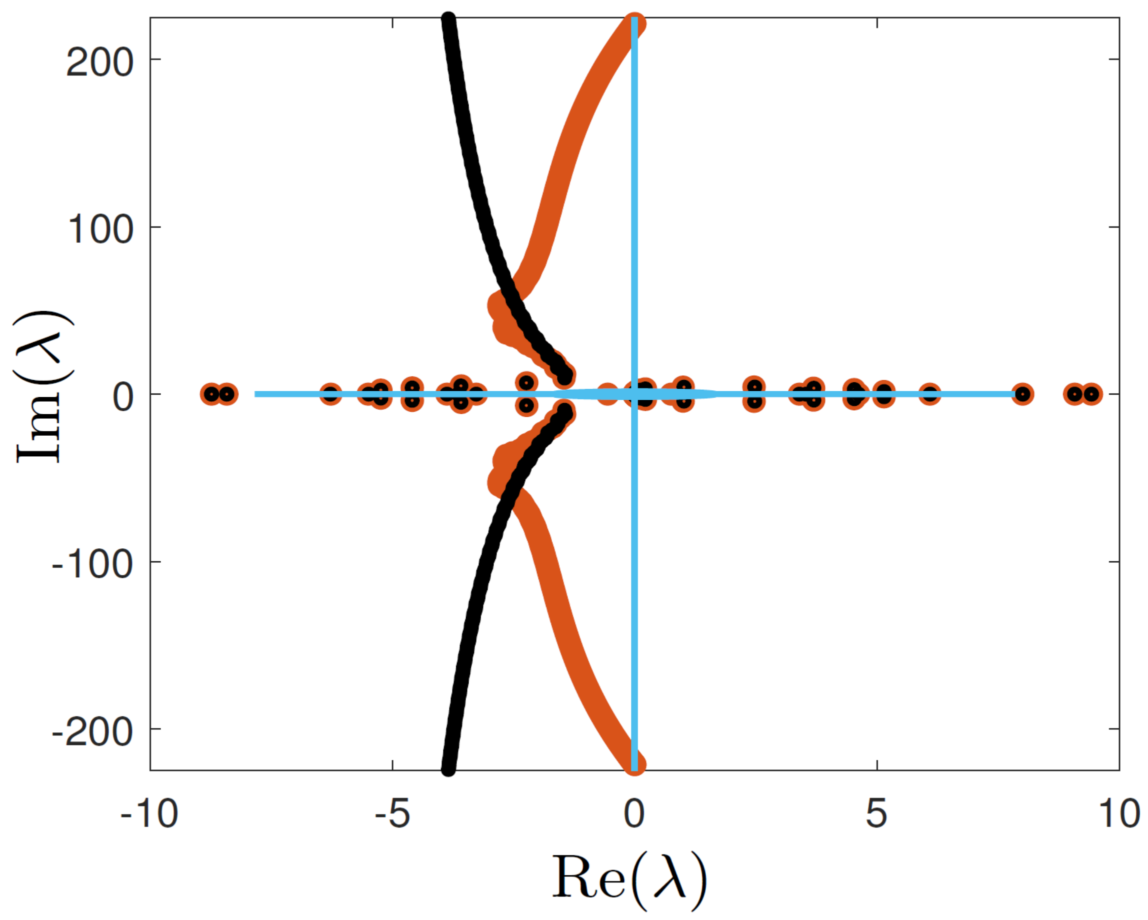


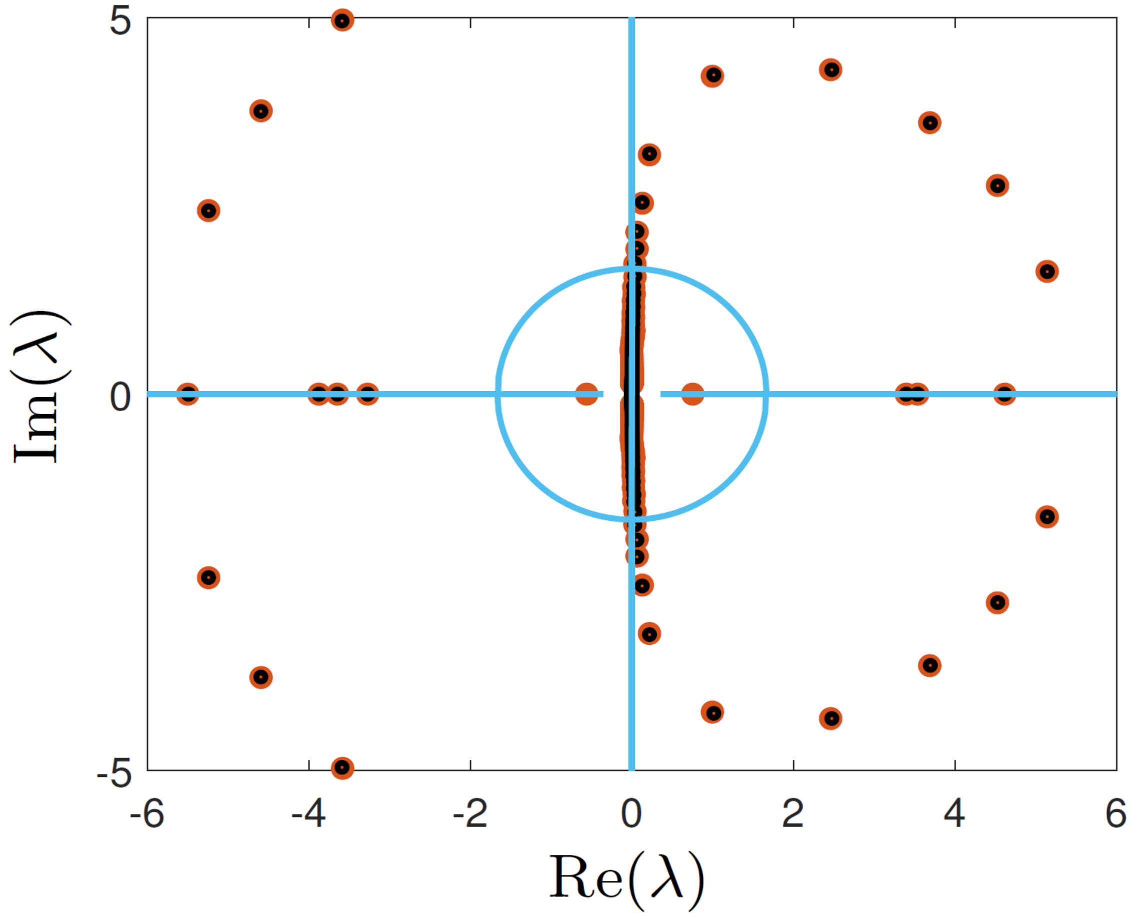
η corresponds to refractive index.

λ correspond to guided and leaky modes.

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

Example: planar waveguide





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

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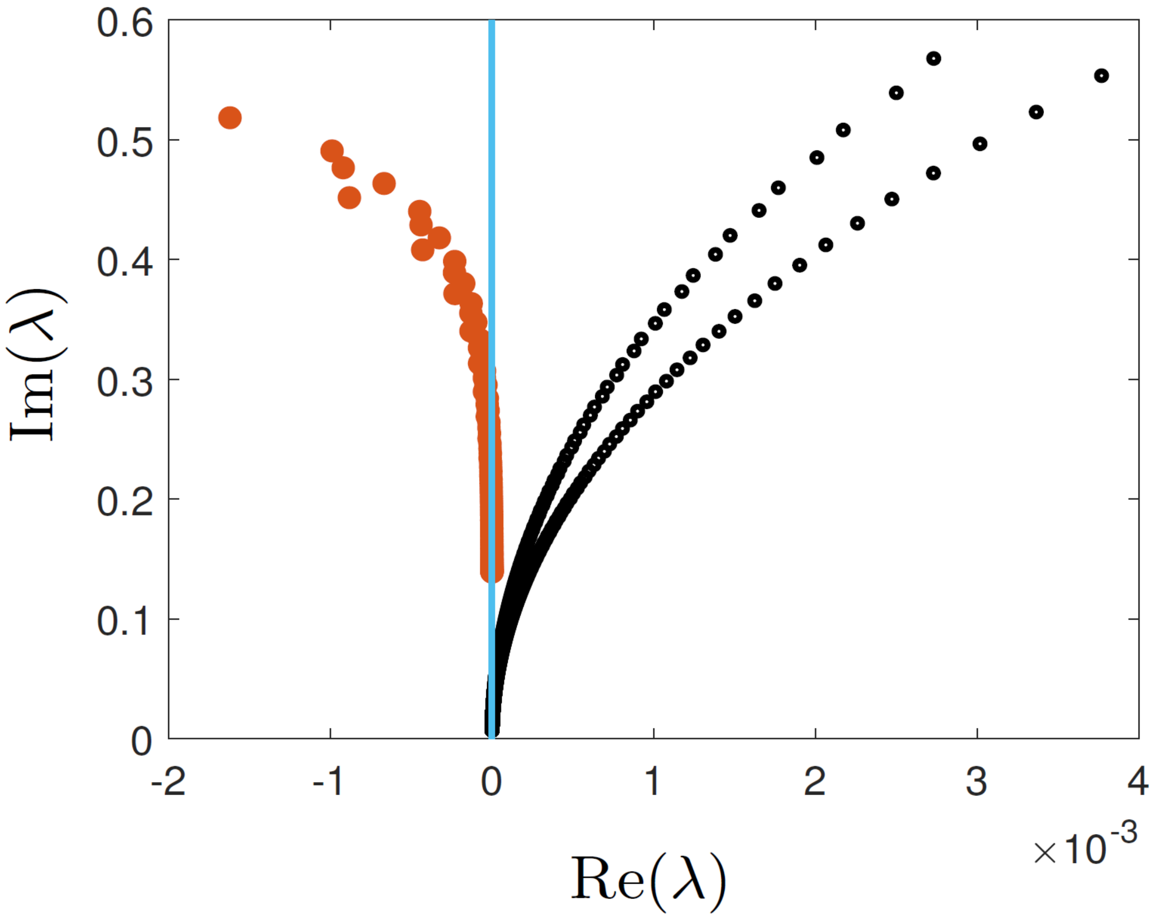

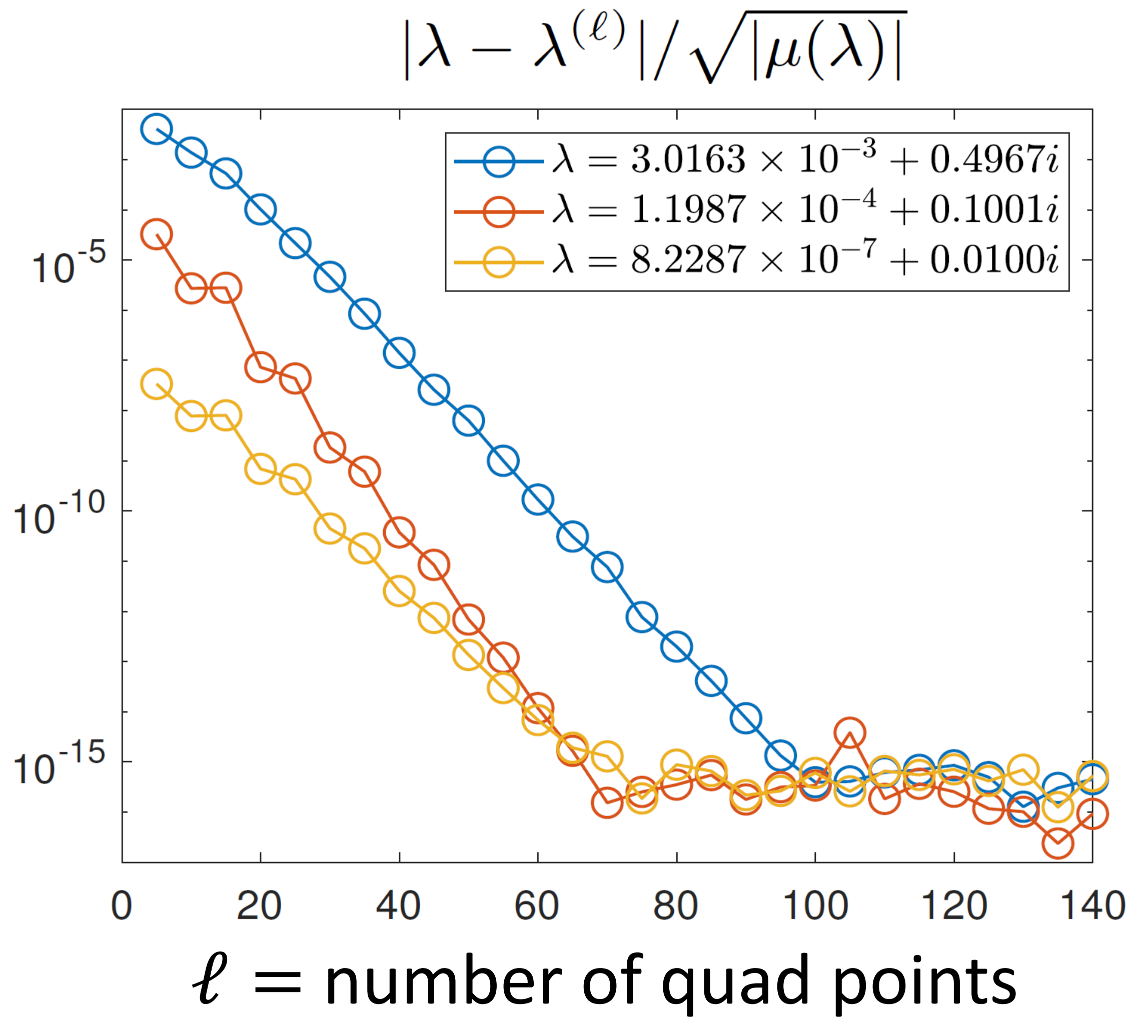

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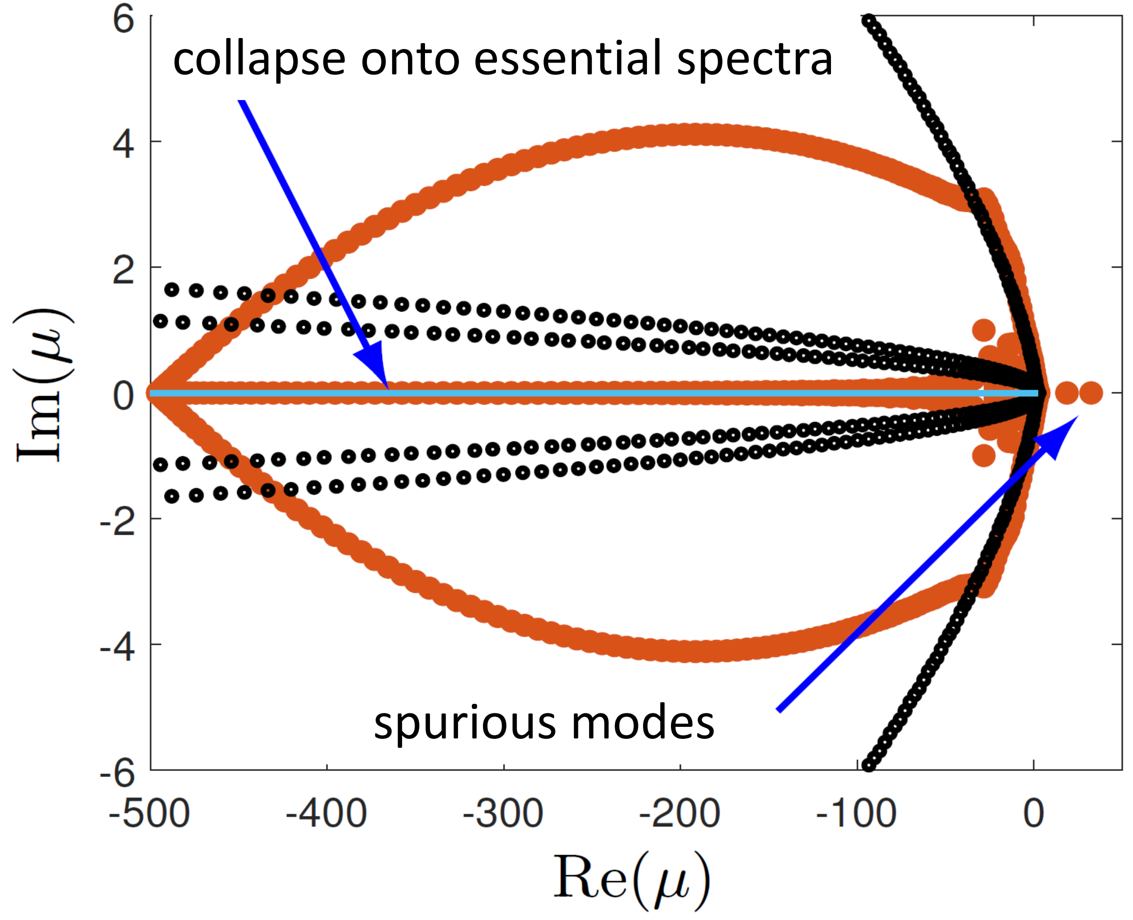
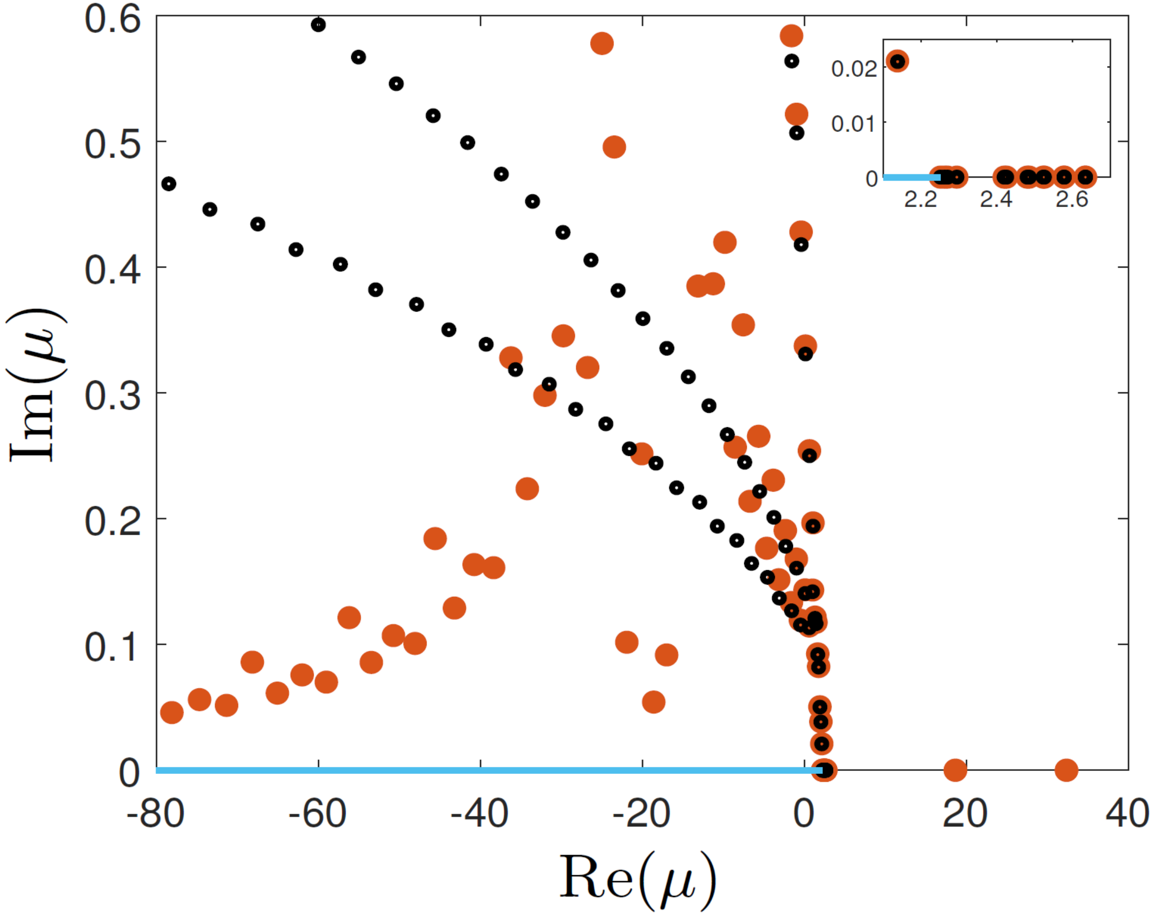




- C., Townsend, *"Avoiding discretization issues for nonlinear eigenvalue problem"*, preprint.

Key Foundations Developments

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

  + Structure of SCI hierarchy allows us to mix and match.
- Leads to universal algorithms for classes of operators.

This framework is now entering computational PDEs, computer-assisted proofs, foundations of AI, and optimization.

Key Algorithmic Developments

- A new suite of "infinite-dimensional" algorithms. **Solve-then-discretise**.
- **Methods built on $\boldsymbol{\sigma_{\mathrm{inf}}(A)}$**, e.g., compute $\sigma_{\mathrm{inf}}(A\mathcal{P}_n^*)$ or $\sqrt{\sigma_{\mathrm{inf}}(\mathcal{P}_n A^* A \mathcal{P}_n^*)}$
  - 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.

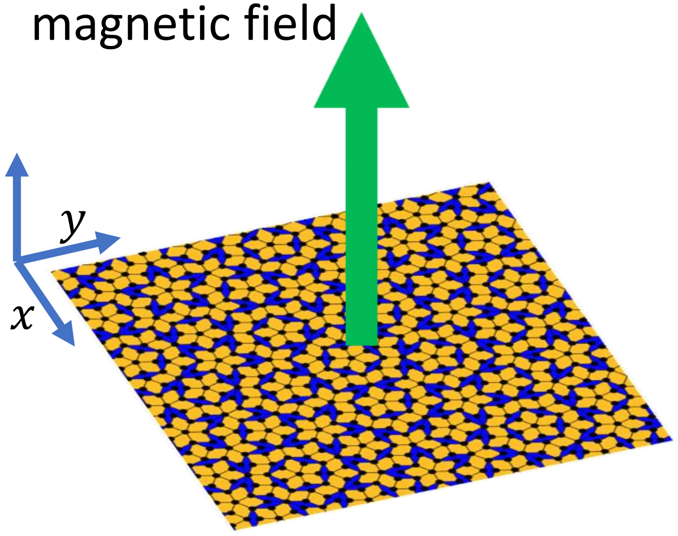
- C., Horning, Townsend "*Computing spectral measures of self-adjoint operators,*" **SIAM Rev.**, 2021.

Open Problems Related to Workshop!

- Structure-preserving infinite-dimensional methods for NEPs.
- Essential spectra of NEPs.
  - Expect $\mathrm{SCI} > 1$ for essential spectra, even if pencil is Hermitian.
- Foundations of data-driven spectral problems.
- Characterising spectral pollution for eigenvalue-dependent boundary conditions (e.g., problems like $\mathtt{acoustic\_wave\_2d}$, polynomial pencils)
- Stability and convergence results for InfBeyn with higher moments.
- Π_1 algorithm (cover) for 2D aperiodic discrete Schrödinger operators.

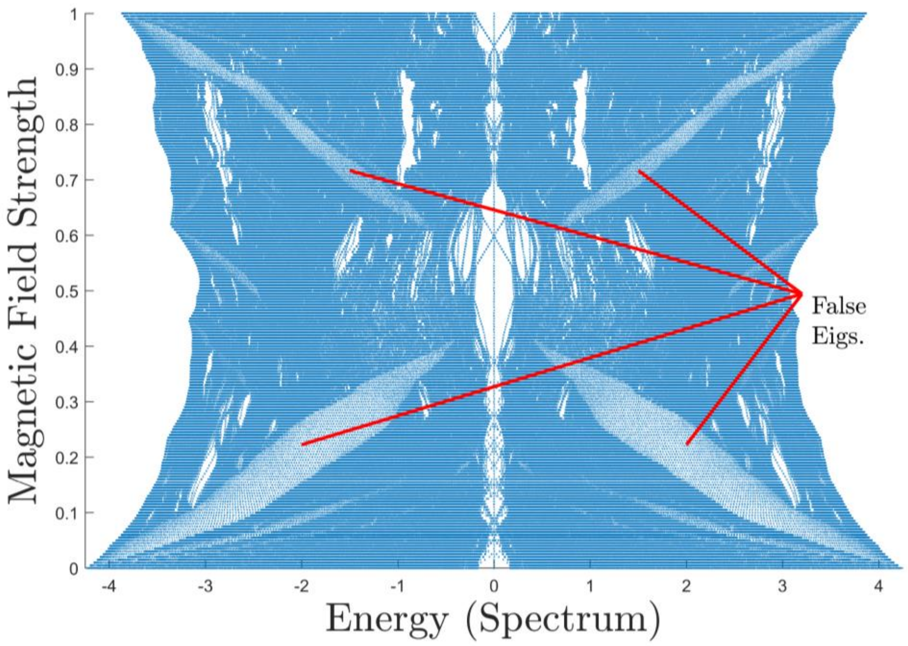
Example: quasicrystals (discrete aperiodic Hamiltonian)

perpendicular magnetic field

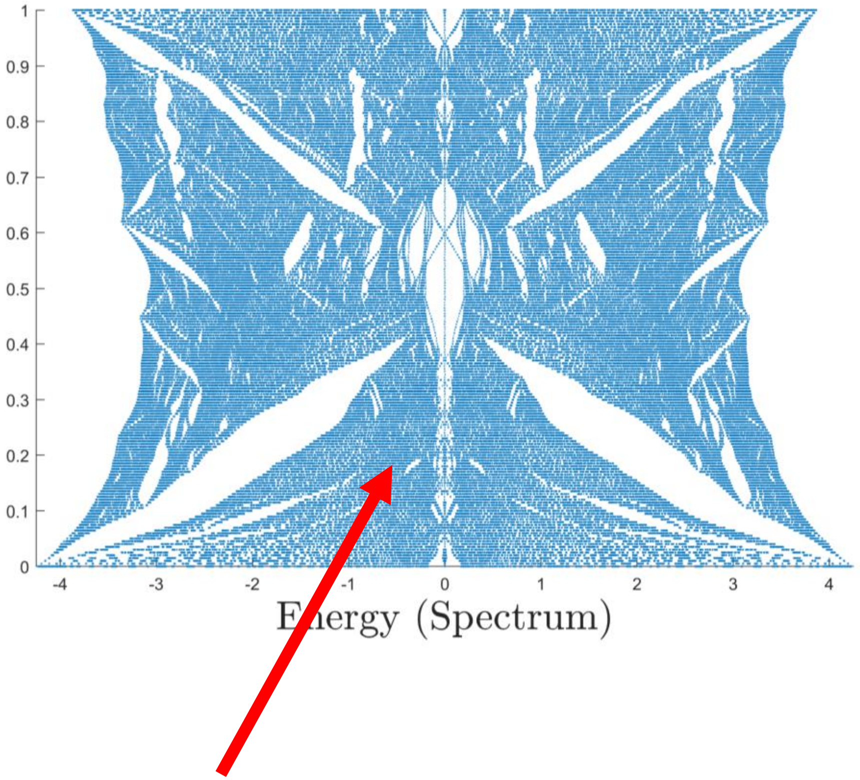


Infinite matrix: discrete Schrödinger operator

Naïve Method



Careful Method



Verified error bounds

- C., Roman, Hansen, “How to compute spectra with error control,” **Phys. Rev. Lett.**,,2019.