

The foundations of infinite-dimensional spectral computations

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#### The infinite-dimensional spectral problem

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

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

Also deal with PDEs, integral operators etc.

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

"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)

## Why spectra?

**Applications:** Quantum mechanics, structural mechanics, optics, acoustics, statistical physics, number theory, matter physics, PDEs, data analysis, neural networks and AI, nuclear scattering, optics, computational chemistry, ...

#### Rich history of **computational spectral theory**:

D. Arnold (Minnesota), W. Arveson (Berkeley), A. Böttcher (Chemnitz), W. Dahmen (South Carolina), E. B. Davies (KCL), P. Deift (NYU), L. Demanet (MIT), M. Embree (Virginia Tech), C. Fefferman (Princeton), G. Golub (Stanford), A. Iserles (Cambridge), I. Ipsen (NCS), S. Jitomirskaya (UCI), A. Laptev (Imperial), L. Lin (Berkeley) M. Luskin (Minnesota), S. Mayboroda (Minnesota), W. Schlag (Yale), E. Schrödinger (DIAS), J. Schwinger (Harvard), N. Trefethen (Oxford), V. Varadarajan (UCLA), S. Varadhan (NYU), J. von Neumann (IAS), M. Zworski (Berkeley), ...

**Interesting pure math application:** Many **computer-assisted proofs** involve spectra. E.g., dynamical systems, hydrodynamics, atomic resonances, etc.

## 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?

<sup>•</sup> Digernes, Varadarajan, Varadhan, "Finite approximations to quantum systems," Rev. Math. Phys., 1994.

#### Warm-up: bounded diagonal operators

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

**Assumption:** Algorithm can query entries of A (e.g., as an oracle in BSS or Turing) **Algorithm:**  $\Gamma_n(A) = \{a_1, a_2, ..., a_n\} \rightarrow \text{Spec}(A) = \overline{\{a_1, a_2, ...\}}$  in Haus. Metric. **One-sided error control:**  $\Gamma_n(A) \subset \text{Spec}(A)$ 

**Optimal:** Can't obtain  $\widehat{\Gamma}_n(A) \to \operatorname{Spec}(A)$  with  $\operatorname{Spec}(A) \subset \widehat{\Gamma}_n(A)$ .

## Example: compact operators (still easy?)

classic method

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

**Algorithm:**  $\Gamma_n(A) = \text{Spec}(P_nAP_n)$  converges to Spec(A) in Haus. Metric. **Question:** Can we verify the output?

i.e., Does there exist  $\widehat{\Gamma}_n(A) \to \operatorname{Spec}(A)$  with  $\widehat{\Gamma}_n(A) \subset \operatorname{Spec}(A) + B_2^{-n}$ ?

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#### Answer: No!

No algorithm can do this on whole class, even for self-adjoint compact operators.

#### What about Jacobi operators?

$$A = \begin{pmatrix} a_1 & b_1 & & \\ b_1 & a_2 & b_2 & \\ & b_2 & a_3 & \ddots \\ & & \ddots & \ddots \end{pmatrix},$$

$$b_k > 0$$
,  $a_k \in \mathbb{R}$ 

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?!

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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.  $\lim_{n \to \infty} \Gamma_n(A) = \operatorname{Spec}(A)$  and  $\Gamma_n(A) \subset \operatorname{Spec}(A) + B_2^{-n}$ ,

for any sparse normal operator A

- C., Roman, Hansen, "How to compute spectra with error control," Phys. Rev. Lett., 2019.
- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," preprint.

#### A curious case of limits

General bounded:

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

**Algorithm:**  $\exists \{\Gamma_{n_3,n_2,n_1}\}$  s.t.  $\lim_{n_3 \to \infty} \lim_{n_2 \to \infty} \lim_{n_1 \to \infty} \Gamma_{n_3,n_2,n_1}(A) = \operatorname{Spec}(A)$ 

**Question:** Can we do better?

- Hansen, "On the solvability complexity index, the *n*-pseudospectrum and approximations of spectra of operators," J. Amer. Math. Soc., 2011.
- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," preprint.
- C., "On the computation of geometric features of spectra of linear operators on Hilbert spaces," Found. Comput. Math., 2022.

#### A curious case of limits

General bounded: 
$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots \\ Algorithm: \exists \{\Gamma_{n_3,n_2,n_1}\} \text{ s.t. } \vdots \text{ and } Anveson's lament! \\ \square_{n_1 \to \infty} r_{n_3,n_2,n_1}(A) = \operatorname{Spec}(A)$$
Question: Can we do by EX.

**Answer:** No! Canonically embed problems such as:

Given  $B \in \{0,1\}^{\mathbb{N} \times \mathbb{N}}$ , does *B* have a column with infinitely many 1's?

#### $\Rightarrow$ lower bound on number of "successive limits" needed (indep. of comp. model).

- Hansen, "On the solvability complexity index, the *n*-pseudospectrum and approximations of spectra of operators," J. Amer. Math. Soc., 2011.
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## Solvability Complexity Index Hierarchy

Class  $\Omega \ni A$ , want to compute  $\Xi: \Omega \to (\mathcal{M}, d)$ 

- $\Delta_0$ : Problems solved in finite time (v. rare for cts problems).
- $\Delta_1$ : Problems solved in "one limit" with full error control:

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

•  $\Delta_2$ : Problems solved in "one limit":

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

•  $\Delta_3$ : Problems solved in "two successive limits":

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

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.

metric space

- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," preprint.
- Hansen, "On the solvability complexity index, the *n*-pseudospectrum and approximations of spectra of operators," J. Amer. Math. Soc., 2011.
- McMullen, "Families of rational maps and iterative root-finding algorithms," Ann. of Math., 1987.
- Doyle, McMullen, "Solving the quintic by iteration," Acta Math., 1989.
- Smale, "The fundamental theorem of algebra and complexity theory," Bull. Amer. Math. Soc., 1981.

# 8/36 Solvability Complexity Index Hierarchy $\lim_{n \to \infty} \lim_{m \to \infty} \Gamma_{n,m}(A) = \Xi(A)$

- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," preprint.
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#### Error control for spectral problems

 $\Sigma_1$  convergence



•  $\Sigma_1$ :  $\exists$  alg. { $\Gamma_n$ } s.t.  $\lim_{n \to \infty} \Gamma_n(A) = \Xi(A), \max_{z \in \Gamma_n(A)} \operatorname{dist}(z, \Xi(A)) \le 2^{-n}$ 

#### Error control for spectral problems



- $\Sigma_1$ :  $\exists$  alg. { $\Gamma_n$ } s.t.  $\lim_{n \to \infty} \Gamma_n(A) = \Xi(A), \max_{z \in \Gamma_n(A)} \operatorname{dist}(z, \Xi(A)) \le 2^{-n}$
- $\Pi_1$ :  $\exists$  alg. { $\Gamma_n$ } s.t.  $\lim_{n \to \infty} \Gamma_n(A) = \Xi(A), \max_{z \in \Xi(A)} \operatorname{dist}(z, \Gamma_n(A)) \le 2^{-n}$

Such problems can be used in a proof!

#### 10/36 Sample: some results for bounded op. on $l^2(\mathbb{N})$ **Increasing difficulty Error control** $\Pi_1$ $\Pi_0$ $\Delta_1 \subseteq \Sigma_1 \cup \Pi_1 \subseteq$ $\Delta_0$ Ç $\zeta_{r}$

 $\Sigma_1$ 

Н

 $\Sigma_0$ 



#### Sample: some results for bounded op. on $l^2(\mathbb{N})$ **Increasing difficulty Error control** $\Pi_2$ $\Pi_1$ $\Pi_0$ Н $\Delta_2 \subseteq \Sigma_2 \cup \Pi_2 \subseteq \Delta_3$ $\Delta_1 \subseteq \Sigma_1 \cup \Pi_1 \subseteq$ Ç $\Delta_0$ C<sub>4</sub> $\Sigma_0$ $\Sigma_1$ $\Sigma_2$

Two limits: SCI  $\leq 2$ 

10/36



Three limits: SCI  $\leq$  3 ...







**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 ...

<sup>•</sup> C., "The foundations of infinite-dimensional spectral computations," PhD diss., University of Cambridge, 2020.

## Why study these foundations?

- SCI > 1 classifications  $\Rightarrow$  tells us assumptions needed to lower SCI.
- $\Sigma_1$  and  $\Pi_1$  classifications  $\implies$  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.

# Example 1: $\Sigma_1$ algorithm for spectra

$$\sigma_{\inf}(T) = \inf\{\|Tv\| \colon v \in \mathfrak{D}(T), \|v\| = 1\}$$

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$$\gamma_{n_1,n_2}(A,z) = \min\{\sigma_{\inf}(P_{n_1}[A-z]P_{n_2}), \sigma_{\inf}(P_{n_1}[A^*-\bar{z}]P_{n_2})\}$$

$$n_{1} \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

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

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$$\gamma_{n_1,n_2}(A,z) \uparrow \gamma_{n_2}(A,z) \coloneqq \min\{\sigma_{\inf}([A-z]P_{n_2}), \sigma_{\inf}([A^*-\bar{z}]P_{n_2})\}, \text{ as } n_1 \to \infty$$



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$$\gamma_{n_2}(A,z) \downarrow \gamma(A,z) \coloneqq \min\{\sigma_{\inf}(A-z), \sigma_{\inf}(A^*-\bar{z})\} = \|(A-z)^{-1}\|^{-1}, \text{ as } n_2 \to \infty$$

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

The three-limit algorithm  

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

$$Spec_{\varepsilon}(A)$$

$$\gamma_{n_1,n_2}(A, z) = \min\{\sigma_{inf}(P_{n_1}[A - z]P_{n_2}), \sigma_{inf}(P_{n_1}[A])$$

$$Spec(A)$$

$$Spec(A)$$

$$\gamma_{n_1,n_2}(A, z) \uparrow \gamma_{n_2}(A, z) \coloneqq \min\{\sigma_{inf}([A - z]P_{n_2}), \sigma_{inf}([A^* - \overline{z}]P_{n_2})\}, as u_1 \to \infty$$

$$\gamma_{n_2}(A, z) \downarrow \gamma(A, z) \coloneqq \min\{\sigma_{inf}(A - z), \sigma_{inf}(A^* - \overline{z})\} = \|(A - z)^{-1}\|^{-1}, as n_2 \to \infty$$

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Approx. pseudospectrum:  $\lim_{n_2 \to \infty} \lim_{n_1 \to \infty} \widehat{\Gamma}_{n_1, n_2}(A, \varepsilon) = \operatorname{Spec}_{\varepsilon}(A) = \{z: \gamma(A, z) \le \varepsilon\}$  $\Gamma_{n_1, n_2, n_3}(A) = \widehat{\Gamma}_{n_1, n_2}(A, 1/n_3)$ 

<sup>•</sup> Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," preprint.

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

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

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

#### What assumptions are needed to reduce the number of limits?

<sup>•</sup> Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," preprint.





#### Aperiodicity $\Rightarrow$ interesting physics but very hard to compute spectra!

Model: Perpendicular magnetic field (of strength *B*).



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#### **Typical approach:** $n \times n$ truncation (possibly with BCs) **Problems:** spectral pollution, which eigenvalues are reliable etc.



#### New approach: $f(n) \times n$ truncation. Naturally captures interactions!

## Sketch of algorithm

$$\sigma_{\inf}(T) = \inf\{\|Tv\|: v \in \mathfrak{D}(T), \|v\| = 1\}$$
$$\|(A - z)^{-1}\|^{-1} = \min\{\sigma_{\inf}(A - z), \sigma_{\inf}(A^* - \overline{z})\}$$
$$\sigma_{\inf}(P_{f(n)}[A - z]P_n) = \sigma_{\inf}([A - z]P_n) \downarrow \sigma_{\inf}(A - z)$$

Suppose we can relate  $||(A - z)^{-1}||^{-1}$  to dist(z, Spec(A)), e.g., normal operators:

$$\sigma_{\inf}(P_{f(n)}[A-z]P_n) \downarrow ||(A-z)^{-1}||^{-1} = \operatorname{dist}(z, \operatorname{Spec}(A))$$
  
**Final ingredient:** local and adaptive search for local minimisers.

Square truncations

Spectral pollution.

#### New method

Convergent computation.





Does not converge No error control Converges Error control

## Example (local uniform convergence)

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

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

- 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

## Example (local uniform convergence)

17/36

Not verifiable

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

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- 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  $\mathbb{R}^d$ . Verifiable Then
- (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  $TV_{[-n,n]^d}(c_k) = O(b_n) \Longrightarrow \{Sp, \Omega\} \in \Delta_2 \setminus (\Sigma_1 \cup \Pi_1).$ 

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





# Example with discrete spectra (verified with interval arithmetic)

 $-\nabla^2 + x^2 + V(x)$  on  $\mathbb{R}$ 

V	$\cos(x)$	tanh( <i>x</i> )	$\exp(-x^2)$	$1/(1 + x^2)$
$E_0$	1.7561051579	0.8703478514	1.6882809272	1.7468178026
$E_1$	3.3447026910	2.9666370800	3.3395578680	3.4757613534
<i>E</i> <sub>2</sub>	5.0606547136	4.9825969775	5.2703748823	5.4115076464
<i>E</i> <sub>3</sub>	6.8649969390	6.9898951678	7.2225903394	7.3503220313
$E_4$	8.7353069954	8.9931317537	9.1953373991	9.3168983920



Example 2:  $\Delta_2$  alg. for spectral meas.

### Spectral measures $\rightarrow$ diagonalisation

• Fin.-dim.:  $B \in \mathbb{C}^{n \times n}$ ,  $B^*B = BB^*$ , o.n. basis of e-vectors  $\{v_j\}_{j=1}^n$ 

$$v = \left[\sum_{j=1}^{n} v_{j} v_{j}^{*}\right] v, \qquad Bv = \left[\sum_{j=1}^{n} \lambda_{j} v_{j} v_{j}^{*}\right] v, \qquad \forall v \in \mathbb{C}^{n}$$

• Inf.-dim.: Operator  $A: \mathcal{D}(A) \to \mathcal{H}$ . Typically, no basis of e-vectors! Spectral theorem: (projection-valued) spectral measure E

$$f = \left[ \int_{\operatorname{Spec}(A)} 1 \, dE(\lambda) \right] f, \qquad Af = \left[ \int_{\operatorname{Spec}(A)} \lambda \, dE(\lambda) \right] f, \qquad \forall f \in \mathcal{H}$$

• Spectral measures:  $\mu_f(U) = \langle E(U)f, f \rangle (||f|| = 1)$  prob. Measure on  $\mathbb{R}$ .

### A two-limit algorithm (Stone's formula)

#### **Smoothed spectral measure:**

$$\mu_f^{\varepsilon}(x) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{\varepsilon \, d\mu_f(\lambda)}{(x-\lambda)^2 + \varepsilon^2} = \frac{\langle [(A - [x + i\varepsilon])^{-1} - (A - [x - i\varepsilon])^{-1}]f, f \rangle}{2\pi i}$$

$$x \rightarrow 0(\varepsilon)$$

$$e^{-i\theta} = \text{"smoothing parameter"}$$

## A two-limit algorithm (Stone's formula)

#### **Smoothed spectral measure:**

$$\mu_f^{\varepsilon}(x) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{\varepsilon \, d\mu_f(\lambda)}{(x-\lambda)^2 + \varepsilon^2} = \frac{\langle [(A - [x + i\varepsilon])^{-1} - (A - [x - i\varepsilon])^{-1}]f, f \rangle}{2\pi i}$$

Discretize RHS with size 
$$n_1$$
, to get  $\mu_{f,n_1}^{\varepsilon}$ . Set  
 $\Gamma_{n_1,n_2}(A) = \mu_{f,n_1}^{1/n_2}$ 



Converges in weak sense.

Without extra assumptions, this is sharp!!

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Converges in weak sense.

Without extra assumptions, this is sharp!!

If we can compute RHS with error control (e.g., residuals), choose  $n_1(\varepsilon)$ .

#### Example: integral operator

$$[Au](x) = xu(x) + \int_{-1}^{1} e^{-(x^2 + y^2)} u(y) dy$$

Discretize using adaptive Chebyshev collocation method.



#### Example: integral operator



Slow convergence (more than five digits infeasible). Can we do better?

## High-order versions of Stone's formula

*m*th order rational "smoothing" kernels:

$$K(x) = \frac{1}{2\pi i} \sum_{j=1}^{m} \frac{\alpha_j}{x - a_j} - \frac{\overline{\alpha_j}}{x - \overline{a_j}}, K_{\varepsilon}(x) = K(x/\varepsilon)/\varepsilon$$

$$\begin{bmatrix} K_{\varepsilon} * \mu_f \end{bmatrix}(x)$$

$$= \frac{-1}{2\pi i} \sum_{j=1}^{m} \langle [\alpha_j (A - [x - \varepsilon a_j])^{-1} - \overline{\alpha_j} (A - [x - \varepsilon \overline{a_j}])^{-1}] f, f$$

 $\Rightarrow$  larger  $\varepsilon$  for a given accuracy  $\Rightarrow$  smaller  $n_1(\varepsilon)$  for a given accuracy



0

Х

2

1.5

0.5

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## Demo: radial Schrödinger

$$[\mathcal{L}u](r) = -\frac{d^2u}{dr^2}(r) + \left(\frac{\ell(\ell+1)}{r^2} + \frac{1}{r}(e^{-r}-1)\right)u(r), \qquad r > 0.$$

#### Demo: radial Schrödinger



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#### **Eigenvalues of Dirac operator**

$$\mathcal{D}_V = egin{pmatrix} 1+V(r) & -rac{d}{dr}+rac{\kappa}{r} \ rac{d}{dr}+rac{\kappa}{r} & -1+V(r) \end{pmatrix}$$



## Spectral measures of self-adjoint operators





Horizontal slice = spectral measure at constant magnetic field strength.

#### Software package

**SpecSolve** available at <u>https://github.com/SpecSolve</u> Capabilities: ODEs, PDEs, integral operators, discrete operators.

## Executive summary of theorems

Input an open (or closed) set

- Generic assumptions: Computing  $(A, f, U) \hookrightarrow \mu_f(U)$  has SCI = 1 but error control or rate *impossible* (even for discrete Schrödinger).
- If spectral measure  $\mu_f$  is a.c. on interval I, with  $\mathcal{C}^{n,\alpha}$  density  $\rho_f$ , then  $\left\|\rho_f \left[K_{\varepsilon} * \mu_f\right]\right\|_{L^{\infty}(I)} = \mathcal{O}(\varepsilon^{n+\alpha} + \varepsilon^m \log(1/\varepsilon))$
- Weak convergence always  $\mathcal{O}(\varepsilon^m \log(1/\varepsilon))$  for  $\mathcal{C}^m$  test functions.
- Splitting into spectral type: SCI = 2 or 3.

NB: Constants can be made  $\underline{explicit} \Rightarrow$  complexity bounds for spec. meas.

<sup>•</sup> C., "Computing spectral measures and spectral types," Comm. Math. Phys., 2021

## Further areas

## Other areas with SCI results

- PDEs e.g.:
  - Can you solve Schrödinger eq. on  $L^2(\mathbb{R}^d)$  with error control?
  - Can you predict blow-up of non-linear PDEs?
- Optimization
- Inverse problems (e.g., imaging)
- Polynomial root-finding: Smale (settled by McMullen), "Is there a purely iterative convergent algorithm for polynomial zero finding?"
- Topology
- As well as ... (computer-assisted proofs, AI, dynamical systems etc.)

## Computer-assisted proof: Dirac-Schwinger conjecture

E(Z) = ground state energy of N: # of electrons, Z: charge of nucleus

$$H = \sum_{k=1}^{N} \left( -\Delta_{x_k} - Z |x_k|^{-1} \right) + \sum_{j < k} |x_j - x_k|^{-1}$$

Theorem: 
$$E(Z) = -c_0 Z^{7/3} + \frac{1}{8} Z^2 - c_1 Z^{5/3} + O(Z^{5/3-1/2835})$$
, as  $Z \to \infty$ 

#### Proof involves spectral analysis, analytic number theory, ..., computer-assisted bound involving solutions of an ODE.

#### Fefferman and Seco implicitly prove $\Sigma_1$ classifications!

- Fefferman, Phong, "On the lowest eigenvalue of a pseudo-differential operator," **Proc. Natl. Acad. Sci. USA**, 1979.
- Fefferman, "The N-body problem in quantum mechanics," Comm. Pure Appl. Math., 1986.
- Fefferman, Seco, "Interval arithmetic in quantum mechanics," Applications of interval computations, 1996.

## Computer-assisted proof: Kepler conjecture (Hilbert's 18th problem)

Proof shows potential counterexamples would satisfy infeasible inequalities

relaxed to  $\approx 10,000$ s linear programs

These can't always be decided!



- Hales, "A proof of the Kepler conjecture," Ann. of Math., 2005.
- Hales et al., "A formal proof of the Kepler conjecture," Forum Math. Pi, 2017.
- Bastounis, Hansen, Vlačić, "The extended Smale's 9th problem," preprint.

Account of Flyspeck project (formal proof)

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#### Example: Barriers of deep learning Smale's 18th problem: "What are the limits of AI?"

**Paradox:** "Nice" linear inverse problems where a *stable* and *accurate* neural network for image reconstruction <u>exists</u>, but it <u>can never be trained</u>!

**Theorem**: Pick positive integers  $n \geq 3$  and M. Class of problems such that:

- (Not trainable) No algorithm (even random) can train a neural network with n digits of accuracy over the dataset with probability greater than 1/2.
- (Not practical) n 1 digits of accuracy possible over the dataset, but any training algorithm requires arbitrarily large training data.
- (Trainable and practical) n 2 digits of accuracy possible over the dataset via training algorithm using *M* training data.

Holds for any architecture, any precision of training data.

#### $\Rightarrow$ Classification theory telling us what can and cannot be done

- C., Antun, Hansen, "The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem," PNAS, 2022.
- Antun, C., Hansen, "Proving Existence Is Not Enough: : Mathematical Paradoxes Unravel the Limits of Neural Networks in Artificial Intelligence," SIAM News, May 2022.
- Choi, "Some AI Systems May Be Impossible to Compute," IEEE Spectrum, March 2022.

## Example: Rigorous Koopmania!

• State  $x \in \Omega \subseteq \mathbb{R}^d$ , **unknown** function  $F: \Omega \to \Omega$  governs dynamics

$$x_{n+1} = F(x_n)$$

- Goal: Learn about system from data  $\{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^{M}$
- Koopman operator  $\mathcal K$  acts on <u>functions</u>  $g:\Omega \to \mathbb C$

 $[\mathcal{K}g](x) = g(F(x))$ 

- $\mathcal K$  is *linear* but acts on an *infinite-dimensional* space.
- Often spectral info encodes the features of the system we want.
- 35,000 papers over last decade, hardly anything on rigorous computation!
- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," preprint.
- C., Ayton, Szőke, "Residual Dynamic Mode Decomposition," preprint.
- Code: <u>https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition</u>

## Summary

SCI hierarchy: a tool that allows us to

- Classify difficulty of continuous and discrete computational problems.
- Prove that algorithms are optimal (in any given computational model).
- Framework ⇒ find assumptions and methods for computational goals.

http://www.damtp.cam.ac.uk/user/mjc249/home.html: slides, papers, and code

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SCI hierarchy: a tool that allows us to

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Shameless advert: you can read more in CUP book out this summer,

"Spectral approximations in infinite dimensions"