

To infinity... and beyond!

The solvability complexity index and 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	\implies	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), C. Fefferman (Princeton), G. Golub (Stanford), A. Iserles (Cambridge), I. Ipsen (NCS), S. Jitomirskaya (UCI), A. Laptev (Imperial), 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),....

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.

Warm-up: bounded diagonal operators

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

Assumption: Algorithm can query entries of *A*.

Algorithm: $\Gamma_n(A) = \{a_1, a_2, ..., a_n\} \rightarrow \text{Spec}(A) = \overline{\{a_1, a_2, ...\}}$ 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: $\Gamma_n(A) = \operatorname{Spec}(P_nAP_n)$ converges to $\operatorname{Spec}(A)$ 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 alg. 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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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.

A curious case of limits

General bounded:
$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots \\ Algorithm: \exists \{\Gamma_{n_3,n_2,n_1}\} \text{ s.t.} \quad \vdots \quad \text{Arveson's lament!} \\ \square (A) = \operatorname{Spec}(A) \\ \square (A) = \operatorname{$$

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 (ind. of comp. model).

- 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., to appear.

Solvability Complexity Index Hierarchy

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

- 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":

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

- 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.

metric space

8/35 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

 Σ_1 convergence



• Σ_1 : \exists alg. { Γ_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



- Σ_1 : \exists alg. { Γ_n } s.t. $\lim_{n \to \infty} \Gamma_n(A) = \Xi(A), \max_{z \in \Gamma_n(A)} \operatorname{dist}(z, \Xi(A)) \le 2^{-n}$
- Π_1 : \exists alg. { Γ_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!

10/35 Sample: some results for bounded op. on $l^2(\mathbb{N})$ **Increasing difficulty Error control** Π_1 Π_0 $\Delta_1 \subseteq \Sigma_1 \cup \Pi_1 \subseteq$ Δ_0 Ç ζ_{r}

 Σ_1

Н

 Σ_0



Sample: some results for bounded op. on $l^2(\mathbb{N})$ **Increasing difficulty Error control** Π_2 Π_1 Π_0 н $\Delta_2 \subseteq \Sigma_2 \cup \Pi_2 \subseteq \Delta_3$ $\Delta_1 \subseteq \Sigma_1 \cup \Pi_1 \subseteq$ Ŷ Δ_0 C₄ Σ_0 Σ_1 Σ_2

Two limits: SCI ≤ 2

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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 ...

[•] 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.
- 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 included as particular cases.

Example 1: Σ_1 algorithm for spectra

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

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

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

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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

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

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

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

$$Spec(A)$$

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

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

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

[•] Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," preprint.

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

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

What assumptions are needed to reduce the number of limits?

[•] 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*).









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.

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Example: quasicrystals

Square truncations

Spectral pollution.

New method

Convergent computation.





Does not converge No error control Converges Error control

Is it right? The importance of verification





- C., Roman, Hansen, "How to compute spectra with error control," Phys. Rev. Lett., 2019.
- Johnstone, C., Nielsen, Öhberg, Duncan, "Bulk Localised Transport States in Infinite and Finite Quasicrystals via Magnetic Aperiodicity," Phys. Rev. B, 2022.

Example (local uniform convergence)

18/35

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

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

- 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)

18/35

Not verifiable

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

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- 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



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



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

Example 2: Δ_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!!

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
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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.

Look at μ_f for $f(x) = \sqrt{3/2}x$ $\mu_f^{\epsilon}(x)$ 10^{2} 10⁰ 10⁻⁴ -2 -1 0 2 1 X

Example: integral operator



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

High-order versions of Stone's formula

 $\overline{\alpha}$.

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



1.5

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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.

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

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 μ_f is a.c. on interval I, with $\mathcal{C}^{n,\alpha}$ density ρ_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 **explicit**.

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 Σ_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)

32/35

Example: Barriers of deep learning

PNAS	৹ ≡	UNIVERSITY OF CAMBRIDGE	Study at Cambridge	About the University	Research at Cambridge
RESEARCH ARTICLE APPLIED MATHEMATICS FULL ACCESS f ¥ in ⊡ ≦ The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem Matthew], Colbrook ● □, Vegard Antun □, and Anders C. Hansen □ Authors Info & Affiliations		 Research / News / Mathematical paradox demonstrates the limits of AI Research Research home News Our people Spotlights About research versearch Business and enterprise Research Mathematical paradox demonstrates the limits of AI 			
March 16, 2022 119 (12) e2107151119 <u>https://doi.org/10.1073/pnas.21071</u>	D IEEE.ORG IEEE XFLORE DIGITAL LIBRARY IEEE STANDARDS MORE SITES IEEE Spectrum for the technology insider	Q Type to sea	rch		
Significance Instability is the Achilles' heel of modern artificial intelligence training algorithms finding unstable neural networks (NNs) de ones. This foundational issue relates to Smale's 18th mathem century on the limits of AI. By expanding methodologies initia	New research suggests there are limitations to what deep neural networks can do BY CHARLES Q. CHOI 30 MAR 2022 4 MIN READ		ty good at recognising when they get things wrong, but ems are not. According to a new study, Al generally suffers due to a century-old mathematical paradox.		
demonstrate limitations on the existence of (even randomized NNs. Despite numerous existence results of NNs with great a only in specific cases do there also exist algorithms that can c classification theory on which NNs can be trained and introdu suitable conditions—are robust to perturbations and expone number of hidden layers.	1000		Cambridge and the University of Oslo say of modern AI and that a mathematical		similarly, A1 algorithms can't exist for certain problems

• C., Antun, Hansen, "The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem," Proc. Natl. Acad. Sci. USA.

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 functions $g:\Omega\to\mathbb C$

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

- $\mathcal K$ 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 NA of this problem!
- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," preprint.
- C., Ayton, Szőke, "Residual Dynamic Mode Decomposition," J. Fluid Mech., under minor rev.
- 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

Additional slides

Problem: hallucinations and instability



"AI generated hallucination", from Facebook and NYU's FastMRI challenge 2020

Instabilities in medical diagnosisOriginal MolePerturbed Mole



Model confidence

Model confidence

From Finlayson et al., "Adversarial attacks on medical machine learning," Science, 2019.

When can we make AI robust and trustworthy?

Example of the limits of deep learning

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>!

E.g., suppose we want to solve (holds for much more general problems)

$$(P_{1}) \quad \operatorname{argmin}_{x \in \mathbb{C}^{N}} F_{1}^{A}(x) \coloneqq \|x\|_{l^{1}_{w}}, \text{ such that } \|Ax - y\|_{l^{2}} \leq \epsilon$$

$$(P_{2}) \quad \operatorname{argmin}_{x \in \mathbb{C}^{N}} F_{2}^{A}(x, y, \lambda) \coloneqq \lambda \|x\|_{l^{1}_{w}} + \|Ax - y\|_{l^{2}}^{2},$$

$$(P_{3}) \quad \operatorname{argmin}_{x \in \mathbb{C}^{N}} F_{3}^{A}(x, y, \lambda) \coloneqq \lambda \|x\|_{l^{1}_{w}} + \|Ax - y\|_{l^{2}}.$$

$$A \in \mathbb{C}^{m \times N} \text{ (modality, } m < N), \qquad S = \{y_{j}\}_{j=1}^{R} \text{ (samples)}$$
Arises when given $y \approx Ax + e$.

Arbitrary precision of training data

In practice, A not known exactly or cannot be stored to infinite precision.

Assume access to: $\{y_{k,n}\}_{k=1}^R$ and A_n (rational approximations, e.g., floats) such that $\|y_{k,n} - y_k\| \le 2^{-n}, \quad \|A_n - A\| \le 2^{-n}, \quad \forall n \in \mathbb{N}.$

Training set for $(A, S) \in \Omega$:

$$\iota_{\mathcal{A},\mathcal{S}} := \{ (y_{k,n}, \mathcal{A}_n) \mid k = 1, \ldots, R \text{ and } n \in \mathbb{N} \}.$$

In a nutshell: allow access to arbitrary precision training data.

Question: Given a collection Ω of (A, S), does there <u>exist</u> a neural network approximating Ξ (solution map of (P_j)), and <u>can it be trained</u> by an algorithm?

Condition numbers

Given $\Omega \subseteq \mathbb{C}^n$, define

$$\operatorname{Act}(\Omega) = \{j: \exists x, y \in \Omega, x_j \neq y_j\}, \qquad \Omega^{\operatorname{Act}} = \{x: \exists y \in \Omega, x_{\operatorname{Act}(\Omega)^c} = y_{\operatorname{Act}(\Omega)^c}\}$$

• Condition of a mapping $\Xi: \widehat{\Omega} \rightrightarrows \mathbb{C}^m$ with $\Omega \subseteq \widehat{\Omega}:$

$$\operatorname{Cond}(\Xi, \Omega) = \sup_{x \in \Omega} \lim_{\varepsilon \to 0_+} \sup_{\substack{x + z \in \Omega^{\operatorname{Act}} \cap \widehat{\Omega} \\ 0 < \|z\|_{\infty} < \varepsilon}} \frac{\operatorname{dist}(\Xi(x + z), \Xi(x))}{\|z\|_{\infty}}$$

• For problems with constraints (e.g., basis pursuit P₁ or LPs)

$$\nu(A, y) = \inf\{\varepsilon \ge 0 : \|\hat{y} - y\|_2, \|\hat{A} - A\| \le \varepsilon, (\hat{A}, \hat{y}) \in \Omega^{\text{Act}} \text{ and infeasible}\}$$
$$C_{\text{FP}}(A, y) = \frac{\max\{\|y\|_2, \|A\|\}}{\nu(A, y)}$$

• Renegar condition number

$$\mu(A, y) = \inf\{\varepsilon \ge 0 : \|\hat{y} - y\|_2, \|\hat{A} - A\| \le \varepsilon, (\hat{A}, \hat{y}) \in \Omega^{Act}, \Xi \text{ multivalued}\}$$
$$C_{RCC}(A, y) = \frac{\max\{\|y\|_2, \|A\|\}}{\mu(A, y)}$$

Theorem: For any of prev. problems, integer $K \ge 3$ and $L \in \mathbb{N}$, \exists a well-conditioned class $\Omega(K)$ of inputs s.t. simultaneously

1. No deterministic alg. can, given a training set $\iota_{A,S} \in \Omega_T$, produce a neural network (NN) ϕ with (1) $\min_{y \in S} \inf_{x^* \in \Xi(A,y)} \|\phi(y) - x^*\|_2 \le 10^{-K} \quad \forall (A,S) \in \Omega(K).$

For any p > 1/2, no random alg. (any model of comp.) can produce a NN ϕ s.t. (1) holds with prob. $\geq p$.

- 2. (a) ∃ deterministic alg. that , given a training set ι_{A,S} ∈ Ω_T, produces a neural network (NN) φ with
 (2) max inf_{y∈S} x^{*}∈Ξ(A,y) ||φ(y) x^{*}||₂ ≤ 10^{-(K-1)} ∀(A,S) ∈ Ω(K).
 (b) However, for any probabilistic Turing Machine that produces such a NN, any M ∈ N and p ∈ [0, N-m/(N+1-m)), there exists a training set ι_{A,S} ∈ Ω_T s.t. ∀y ∈ S
 P(inf_{x^{*}∈Ξ(A,y)} ||φ(y) x^{*}||₂ > 10^{-(K-1)} or size of training data to construct φ exceeds M) > p.
- 3. \exists deterministic alg. that, given a training set $\iota_{A,S} \in \Omega_T$, produces a NN ϕ accessing at most L training samples of $\iota_{A,S}$ s.t.

(3)
$$\max_{y \in S} \inf_{x^* \in \Xi(A,y)} \|\phi(y) - x^*\|_2 \le 10^{-(K-2)} \quad \forall (A,S) \in \Omega(K).$$

• C., Antun, Hansen, "The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem," **Proc. Natl. Acad. Sci. USA**.

Theorem: For any of prev. problems, integer $K \geq 3$ and $L \in \mathbb{N}$, \exists a well-conditioned class $\Omega(K)$. of inputs s.t. simultaneously No deterministic alg. can, given a training set $\iota_{A,S} \in \Omega_T$, produce a neural network (NN) ϕ with 1. (1) $\min_{y \in S} \inf_{x^* \in \Xi(A, y)} \|\phi(y) - x^*\|_2 \le 10^{-K} \quad \forall (A, S) \in \Omega(K).$ For any p > 1/2, no random alg. (any model of comp.) can produce a NN ϕ s.t. (1) holds with prob. $\geq p$. (a) \exists deterministic alg. that , given a training set $\iota_{A,S} \in \Omega_T$, produces a neural network (NN) ϕ with 2. $\max \inf_{y \in \Omega} \|\phi(y) - x^*\|_2 \le 10^{-(K-1)} \quad \forall (A, S) \in \Omega(K).$ (2) Holds for any architecture, any precision of training data. \Rightarrow Classification theory telling us what can and cannot be done $\mathbb{P}\left(\inf_{x^*\in\Xi(A,V)} \|\phi(y) - x^*\|_2 > 10^{-(K-1)} \text{ or size of training data to construct } \phi \text{ exceeds } M\right)$ > p. \exists deterministic alg. that, given a training set $\iota_{A,S} \in \Omega_T$, produces a NN ϕ accessing at most L 3. training samples of $\iota_{A,S}$ s.t. $\max_{y \in S} \inf_{x^* \in \Xi(A, y)} \|\phi(y) - x^*\|_2 \le 10^{-(K-2)}$ $\forall (A,S) \in \Omega(K).$ (3)

 C., Antun, Hansen, "The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem," Proc. Natl. Acad. Sci. USA.

The world of neural networks



Given a problem and conditions, where does it sit in this diagram?
The world of neural networks



Given a problem and conditions, where does it sit in this diagram?

Example counterpart theorem

Certain conditions: <u>stable</u> neural networks <u>trained</u> with <u>exponential accuracy</u>. E.g., *approximate Łojasiewicz-type inequality*:

> (1) $\min_{x \in \mathbb{C}^N} f(x)$ s.t. $||Ax - y|| \le \varepsilon$ dist(x, solution) $\le \alpha([f(x) - f^*] + [||Ax - y|| - \varepsilon] + \delta)$

Fast Iterative **RE**started **NET**works (FIRENETs) (unrolled primal-dual with novel restart scheme)

Theorem: Training algorithm that, under above assumption, produces *stable* neural networks φ_n of width O(N), depth O(n), guaranteed worst bound

dist($\varphi_n(y)$, solution) $\leq e^{-n} + \delta$

[•] 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.

C., "WARPd: A linearly convergent first-order method for inverse problems with approximate sharpness conditions," SIAM J. Imaging Sci., 2022.

Numerical example of GHA

Image

Fourier Sampling

Walsh Sampling



Figure: Images corrupted with 2% Gaussian noise and reconstructed using 15% sampling.

Numerical example of GHA



Example of severe instability



• Zhu et al., "Image reconstruction by domain-transform manifold learning," Nature, 2018.

MRI: discrete 2D

• Antun et al., "On instabilities of deep learning in image reconstruction and the potential costs of AI," PNAS, 2020.

FIRENET: provably stable (even to adversarial examples) and accurate



Key pillars: stability and accuracy



U-Net with no noise: accurate but unstable



U-Net with noise: stable but inaccurate



FIRENET: balances stability and accuracy?



FIRENET: balances stability and accuracy?



Open problem: use the toolkit to precisely prove theorems about *optimal* trade-offs.



Stabilising unstable neural networks



Data-driven dynamical systems

• 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 $\{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^{M}$
 - E.g., data from trajectories, experimental measurements, simulations, ...
 - E.g., used for forecasting, control, design, understanding, ...
- Applications: chemistry, climatology, electronics, epidemiology, finance, fluids, molecular dynamics, neuroscience, plasmas, robotics, video processing, ...



Operator viewpoint

• Koopman operator $\mathcal K$ acts on functions $g:\Omega \to \mathbb C$

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

• $\mathcal K$ is *linear* but acts on an *infinite-dimensional* space.



• Work in $L^2(\Omega, \omega)$ for positive measure ω , with inner product $\langle \cdot, \cdot \rangle$.

• Koopman, "Hamiltonian systems and transformation in Hilbert space," Proceedings of the National Academy of Sciences, 1931.

• Koopman, v. Neumann, "Dynamical systems of continuous spectra," Proceedings of the National Academy of Sciences, 1932.

Build the matrix



Given dictionary $\{\psi_1, \dots, \psi_{N_K}\}$ of functions $\psi_j: \Omega \to \mathbb{C}$

 $\mathcal{K} \longrightarrow \mathbb{K} = (\Psi_X^* W \Psi_X)^{-1} \Psi_X^* W \Psi_Y \in \mathbb{C}^{N_K \times N_K}$

Residual DMD: Approx. $\mathcal{K} \operatorname{and} \mathcal{K}^* \mathcal{K}$

$$\langle \psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \, \psi_k(x^{(m)}) = \left[\underbrace{\Psi_X^* W \Psi_X}_G \right]_{jk}$$

$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \, \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \left[\underbrace{\Psi_X^* W \Psi_Y}_{K_1} \right]_{jk}$$

$$\langle \mathcal{K}\psi_k, \mathcal{K}\psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(y^{(m)})} \, \psi_k(y^{(m)}) = \left[\underbrace{\Psi_Y^* W \Psi_Y}_{K_2} \right]_{jk}$$

Residuals:
$$g = \sum_{j=1}^{N_K} \mathbf{g}_j \psi_j$$
, $\|\mathcal{K}g - \lambda g\|^2 \approx \mathbf{g}^* [K_2 - \lambda K_1^* - \overline{\lambda} K_1 + |\lambda|^2 G] \mathbf{g}$

- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems,"
 Communications on Pure and Applied Mathematics, under review.
- Code: <u>https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition</u>

Example: Trustworthy computation for large \boldsymbol{d}



• C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," preprint.

-0.4

-0.6

-0.8

-0.1

-0.15

-0.2

-0.25

-0.04

-0.06

-0.08

Example: Trustworthy computation for large \boldsymbol{d}



C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," preprint.

Example: Verify the dictionary

- Reynolds number $\approx 6.4 \times 10^4$
- Ambient dimension (d) ≈ 100,000 (velocity at measurement points)

*Raw measurements provided by Máté Szőke (Virginia Ter

 $\lambda = 0.9439 + 0.2458i$, error ≤ 0.0765







• C., Ayton, Szőke, "Residual Dynamic Mode Decomposition," J. Fluid Mech., under minor rev.

y1/2

 $\operatorname{Im}(\gamma)$

.δ

Example: molecular dynamics (Adenylate Kinase)

Adenylate Kinase



• C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," preprint.

 \bigcirc

2

3

Example: Trustworthy Koopman mode decomposition



• C., Ayton, Szőke, "Residual Dynamic Mode Decomposition," J. Fluid Mech., under minor rev.

Bulk localised transport



 Johnstone, C., Nielsen, Öhberg, Duncan, "Bulk Localised Transport States in Infinite and Finite Quasicrystals via Magnetic Aperiodicity," Phys. Rev. B, 2022.







narios where we can prove that stable and https://publications.jrc.ec.europa.eu/ sitory/handle/JRC119336

ai-versus-md

accurate NNs exist?

nevus, along with the diagnostic probability computed by a deep neural network (NN). 1d. Combined image of the nevus with expedited impossibility slight perturbation and the diagnostic probability from the same https://www.newyorker. deep NN. One diagnosis is clearly incorrect, but can an algo determine which one? Figures 1a and 1b are courtesy of the 2020 agazine/2017/04/03/ fast/MRI Challenge [10], and 1c and 1d are courtesy of [6].