

The Foundations of Infinite-Dimensional Spectral Computations

Matthew Colbrook

University of Cambridge



{BECMC}²⁰

Collaborators during course of PhD:

Jonathan Ben-Artzi (Cardiff)

Anders Hansen (Cambridge)

Andrew Horning (Cornell)

Olavi Nevanlinna (Aalto)

Bogdan Roman (Cambridge)

Markus Seidel (West Saxon)

Alex Townsend (Cornell)

More than just a really big eigenvalue problem!

In discrete setting, operator acting on $\ell^2(\mathbb{N})$:

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots \\ a_{21} & a_{22} & a_{23} & \dots \\ a_{31} & a_{32} & a_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad (Ax)_j = \sum_{k \in \mathbb{N}} a_{jk} x_k.$$

In cts setting, deal with differential operators, integral operators etc.

Finite Case	Infinite Case
Eigenvalues \Rightarrow	Spectrum $\text{Sp}(A) = \{z \in \mathbb{C} : A - z \text{ not bounded invertible}\}$
Eigenvectors \Rightarrow	Spectral Measure (normal case)

Goal: compute spectral properties of the operator from matrix elements, PDE coefficients, or other suitable information.

MUCH harder and more subtle than finite dimensions!

Many applications: quantum mechanics, chemistry, matter physics, statistical mechanics, optics, number theory, PDEs, mathematics of information etc.

Mathematicians and physicists contributing to computational spectral theory form a vast set including many “heavyweights”:

D. Arnold (Minnesota), W. Arveson (Berkeley), A. Böttcher (Chemnitz), W. Dahmen (South Carolina), E. B. Davies (King's College London), P. Deift (NYU), L. Demanet (MIT), C. Fefferman (Princeton), G. Golub (Stanford), A. Iserles (Cambridge), 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),...

But the problem is **notoriously** hard...

Example: Bounded Diagonal Operators (Very Easy)

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

If $\Gamma_n(A) = \{a_1, \dots, a_n\}$ then $\Gamma_n(A) \rightarrow \text{Sp}(A)$ in Hausdorff metric.

Also have $\Gamma_n(A) \subset \text{Sp}(A)$.

This is optimal from a computational foundations point of view.

Example: Compact Operators (Still Easy)

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots \\ a_{21} & a_{22} & a_{23} & \dots \\ a_{31} & a_{32} & a_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \text{ compact}$$

If $\Gamma_n(A) = \text{Sp}(P_n A P_n)$, then $\Gamma_n(A) \rightarrow \text{Sp}(A)$ in Hausdorff metric.

Known for decades.

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Q: Can we gain error control as before?

No! No algorithm can gain error control on the whole class, even for self-adjoint compact operators.

What about Jacobi operators?

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

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New result: Large class Ω (covering arguably most applications and including sparse normal) such that we can compute $\Gamma_n(A) \rightarrow \text{Sp}(A)$ and $E_n(A) \downarrow 0$ for $A \in \Omega$ with

$$\text{dist}(z, \text{Sp}(A)) \leq E_n(A), \quad \forall z \in \Gamma_n(A).$$

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Paradox: Easier problem than compact operators!

Foundations of Infinite-Dimensional Spectral Computations

How: Deal with operators directly, instead of previous 'truncate-then-solve'

⇒ Compute many spectral properties for the first time.

Framework: Classify problems in a computational hierarchy (the SCI hierarchy) measuring their difficulty and the optimality of algorithms.¹

⇒ Algorithms that realise the boundaries of what computers can achieve.

Common theme in examples of this talk: use the resolvent $(A - z)^{-1}$

¹Also has deep connections with logic and descriptive set theory: C. Preprint (2019)

Example 1

Compute the resolvent norm $\gamma(z) := \|(A - z)^{-1}\|^{-1}$



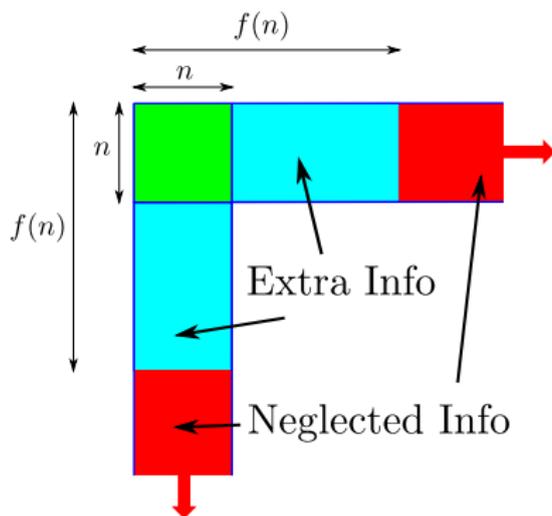
Compute spectra of “most” operators with error control.

M.J. Colbrook, B. Roman, and A.C. Hansen. “How to compute spectra with error control.” *Physical Review Letters* 122(25), 250201 (2019).

Definition (Dispersion: off-diagonal decay)

Dispersion of A bounded by function $f : \mathbb{N} \rightarrow \mathbb{N}$ and null sequence $\{c_n\}$ if

$$\max\{\|(I - P_{f(n)})AP_n\|, \|P_nA(I - P_{f(n)})\|\} \leq c_n.$$



Definition (Controlled growth of the resolvent: well-conditioned)

Continuous increasing function $g : [0, \infty) \rightarrow [0, \infty)$ with $g(x) \leq x$.
Controlled growth of the resolvent by g if

$$g(\text{dist}(z, \text{Sp}(A))) \leq \|(A - z)^{-1}\|^{-1} \quad \forall z \in \mathbb{C}.$$

- Measures conditioning of the problem through

$$\{z \in \mathbb{C} : \|(A - z)^{-1}\|^{-1} \leq \epsilon\} =: \text{Sp}_\epsilon(A) = \bigcup_{\|B\| \leq \epsilon} \text{Sp}(A + B).$$

- Normal operators (A commutes with A^*) well-conditioned with

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Theorem (C., Roman, Hansen. PRL (2019))

Know $f, g \Rightarrow$ can compute $\text{Sp}(A)$ with error control.

Step 1: Approximate locally via smallest singular value:

$$\gamma_n(z) := \min\{\sigma_1(P_{f(n)}(A - z)P_n), \sigma_1(P_{f(n)}(A^* - \bar{z})P_n)\} + c_n.$$

This converges locally uniformly down to $\gamma(z) = \|(A - z)^{-1}\|^{-1}$.

Step 2: Bound the distance to the spectrum:

$$\gamma(z) \leq \text{dist}(z, \text{Sp}(A)) \leq g^{-1}(\gamma(z)) \leq g^{-1}(\gamma_n(z)).$$

Step 3: Find (almost) local minimisers and output $\Gamma_n(A)$ with

$$\Gamma_n(A) \rightarrow \text{Sp}(A), \quad \text{dist}(z, \text{Sp}(A)) \leq g^{-1}(\gamma_n(z)), \quad \sup_{z \in \Gamma_n(A)} g^{-1}(\gamma_n(z)) \rightarrow 0$$

NB: Without either f or g , constructing an algorithm convergent to the spectrum is impossible (even dropping error control).

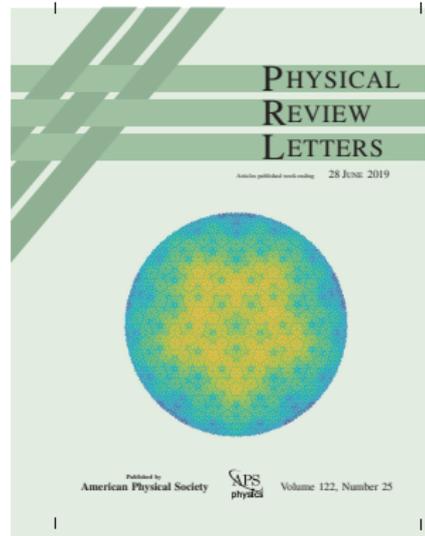
New exemplar of spectral computation?

Method is:

- Local and parallelisable.
- Convergent for first time.
- Explicitly bounds the error:

$$\text{Error} \leq a_n \downarrow 0.$$

- Optimal from foundations point of view.

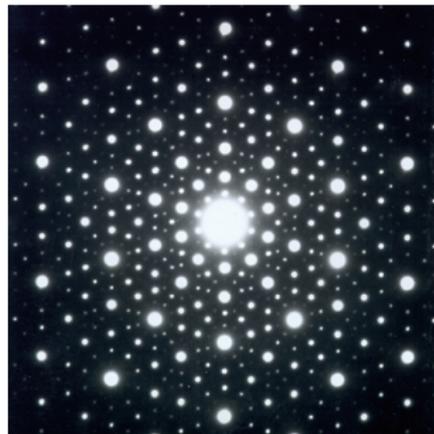


Extends to unbounded operators and PDEs with coefficients of locally bounded total variation (e.g. algorithms point sample coefficients).

NB: Was an open problem since Schwinger's work in the 1960s to do this for general Schrödinger operators (even without error control).

Paradox: Easier problem than compact operators!

Example: Operators in condensed matter physics



Left: Dan Shechtman, **Nobel Prize in Chemistry 2011** for discovery of quasicrystal. Right: Diffraction pattern of a quasicrystal.

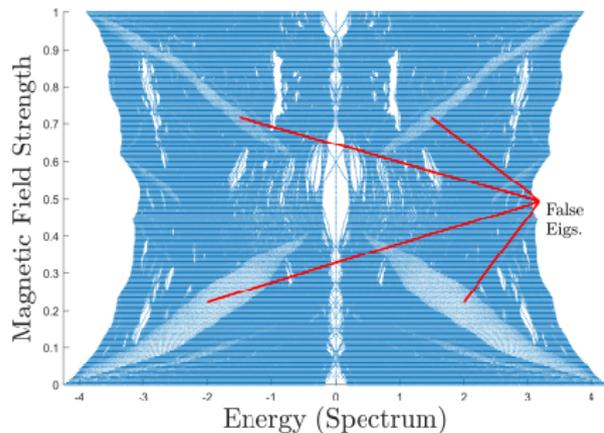
Magnetic properties of quasicrystal.

Hard problem - no previous method even converges to spectrum.

Example: Operators in condensed matter physics

Finite truncations

False 'solutions'.



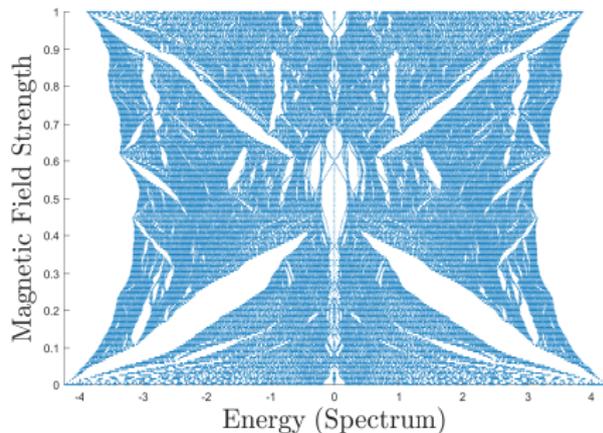
Unreliable

Does not converge

No error control

Infinite-dimensional techniques

First convergent computation.



Reliable

Converges

Error control

Example 2 (Assume A self-adjoint)

Compute resolvent $(A - z)^{-1}\mathbf{x}$ for $\text{Im}(z) > 0$



Compute spectral measures of general self-adjoint operators -
'diagonalisation.'

M.J. Colbrook. "Computing spectral measures and spectral types." arXiv preprint arXiv:1908.06721.

M.J. Colbrook, A. Horning, and A. Townsend. "Computing spectral measures of self-adjoint operators." arXiv preprint arXiv:2006.01766.

If A normal, associated projection-valued measure E^A s.t.

$$A\mathbf{x} = \int_{\text{Sp}(A)} \lambda dE^A(\lambda)\mathbf{x}, \quad \forall \mathbf{x} \in \mathcal{D}(A),$$

Allows computation of functional calculus, has interesting physics etc.

Crucial in: quantum mechanics, scattering in particle physics, correlation in stochastic processes/signal-processing, fluid stability, resonances, density-of-states in materials science, orthogonal polynomials, random matrix theory, evolution PDEs,...

Problem: current methods restricted to operators with lots of structure (typically small perturbations of trivial cases)

Idea: Use the formula

$$\frac{(A - zI)^{-1} - (A - \bar{z}I)^{-1}}{2\pi i} = \int_{\text{Sp}(A)} P(\text{Re}(z) - \lambda, \text{Im}(z)) dE^A(\lambda),$$

$P(x, \epsilon) = \epsilon\pi^{-1}/(x^2 + \epsilon^2)$: convolution with Poisson kernel.

Smoothed version of measure.

Suppose we compute with a truncation parameter n ...

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Theorem (C. (2019))

Know $f \Rightarrow$ can compute measure in one limit.

This is through a rectangular least squares type problem that computes $(A - zI)^{-1}\mathbf{x}$ with (asymptotic) error control. Balance n and ϵ adaptively.

Accelerating convergence with rational kernels

Idea: Replace Poisson kernel with rational kernel

$$K^\epsilon(x) = \frac{1}{2\pi i} \sum_{j=1}^{n_1} \frac{\alpha_j}{x - \epsilon a_j} - \frac{1}{2\pi i} \sum_{j=1}^{n_2} \frac{\beta_j}{x - \epsilon b_j}.$$

Can compute convolution with error control through

$$\begin{aligned} & \langle dE * K^\epsilon \mathbf{x}, \mathbf{y} \rangle(x) \\ &= \frac{1}{2\pi i} \left[- \sum_{j=1}^{n_1} \alpha_j \langle (A - (x - \epsilon a_j))^{-1} \mathbf{x}, \mathbf{y} \rangle + \sum_{j=1}^{n_2} \beta_j \langle (A - (x - \epsilon b_j))^{-1} \mathbf{x}, \mathbf{y} \rangle \right]. \end{aligned}$$

Theorem (C., Horning, Townsend (2020))

Assuming enough local regularity,

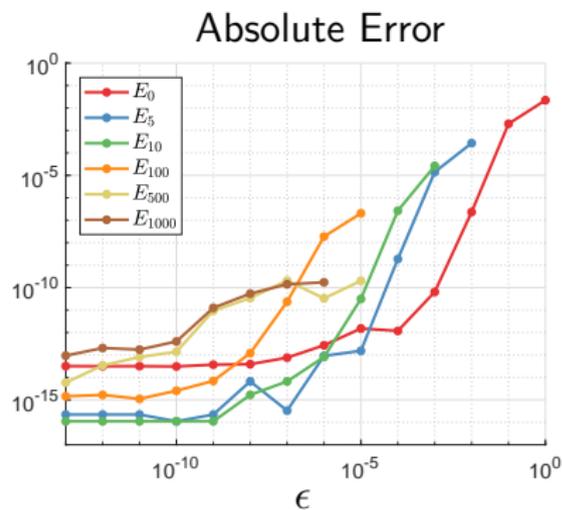
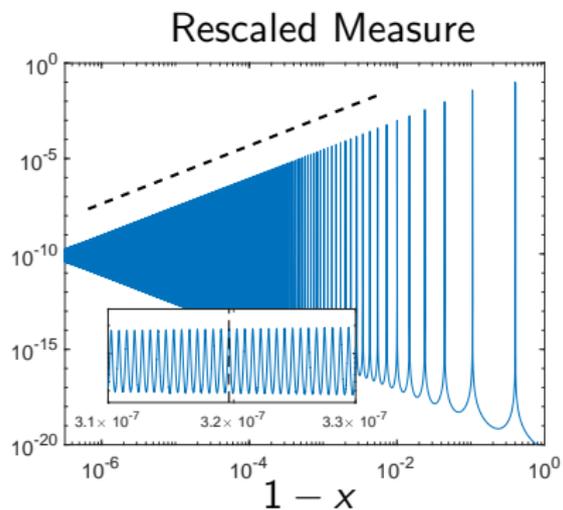
if $j = 1, \dots, m$ moments of K vanish \Rightarrow error is $\mathcal{O}(\epsilon^m)$ (pointwise & L^p_{loc})

Eigenvalue hunting without spectral pollution

Example: Dirac operator.

- Describes the motion of a relativistic spin-1/2 particle.
- Essential spectrum given by $\mathbb{R} \setminus (-1, 1) \Rightarrow$ spectral pollution!
- Consider radially symmetric potential...

Eigenvalue hunting without spectral pollution



NB: Previous state-of-the-art achieves a few digits for a few excited states.

Results in this talk:

- Can compute spectra of a large class of operators with error control. New algorithm is fast, local and parallelisable.
- Can compute spectral measures and spectral decompositions through resolvent. Can be combined with state-of-the-art PDE methods.

Also have foundations for: spectral type (pure point, absolutely continuous, singularly continuous), Lebesgue measure and fractal dimensions of spectra, discrete spectra, essential spectra, eigenvectors + multiplicity, spectral radii, essential numerical ranges, geometric features of spectrum (e.g. capacity), spectral gap problem, ...

For papers, classifications in the SCI hierarchy and numerical code:

<http://www.damtp.cam.ac.uk/user/mjc249/home.html>

Ongoing and future work: foundations of computational PDEs, foundations of (stable) neural networks, and computer-assisted proofs.

Code: high-performance numerical package with resolvent based algorithms for spectral measures (with Andrew Horning):

<https://github.com/SpecSolve/SpecSolve>

References for this program

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