The Foundations of Infinite-Dimensional Spectral Computations

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The infinite-dimensional 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 continuous setting, deal with PDEs, integral operators etc.

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

Goal: compute spectral properties of the operator from matrix elements.

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:

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).

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"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 [to the spectrum], and this raises the question of how to implement the methods of finite dimensional numerical linear algebra to compute the spectra of infinite dimensional operators. 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 techniques."

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Partial answer: can compute spectra of general bounded operators on $\ell^2(\mathbb{N})$ (in Hausdorff metric) using three successive limits[1]

$$\lim_{n_3\to\infty} \lim_{n_2\to\infty} \lim_{n_1\to\infty} \Gamma_{n_3,n_2,n_1}(A) = \mathrm{Sp}(A).$$

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Q: What assumptions do we need to make it easier?

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Example: Bounded Diagonal Operators (Very Easy)

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

If $\Gamma_n(A) = \{a_1, ..., a_n\}$ then $\Gamma_n(A) \to \mathrm{Sp}(A)$ in Hausdorff metric.

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

This is optimal from a foundations point of view.

Example: Compact Operators (Still Easy)

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

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

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Q: Can we gain error control as before?

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Q: Can we gain error control as before?

No algorithm can gain error control on the whole class (even for self-adjoint).

What about Jacobi operators?

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

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

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

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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'

$\Rightarrow$ 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.[2]

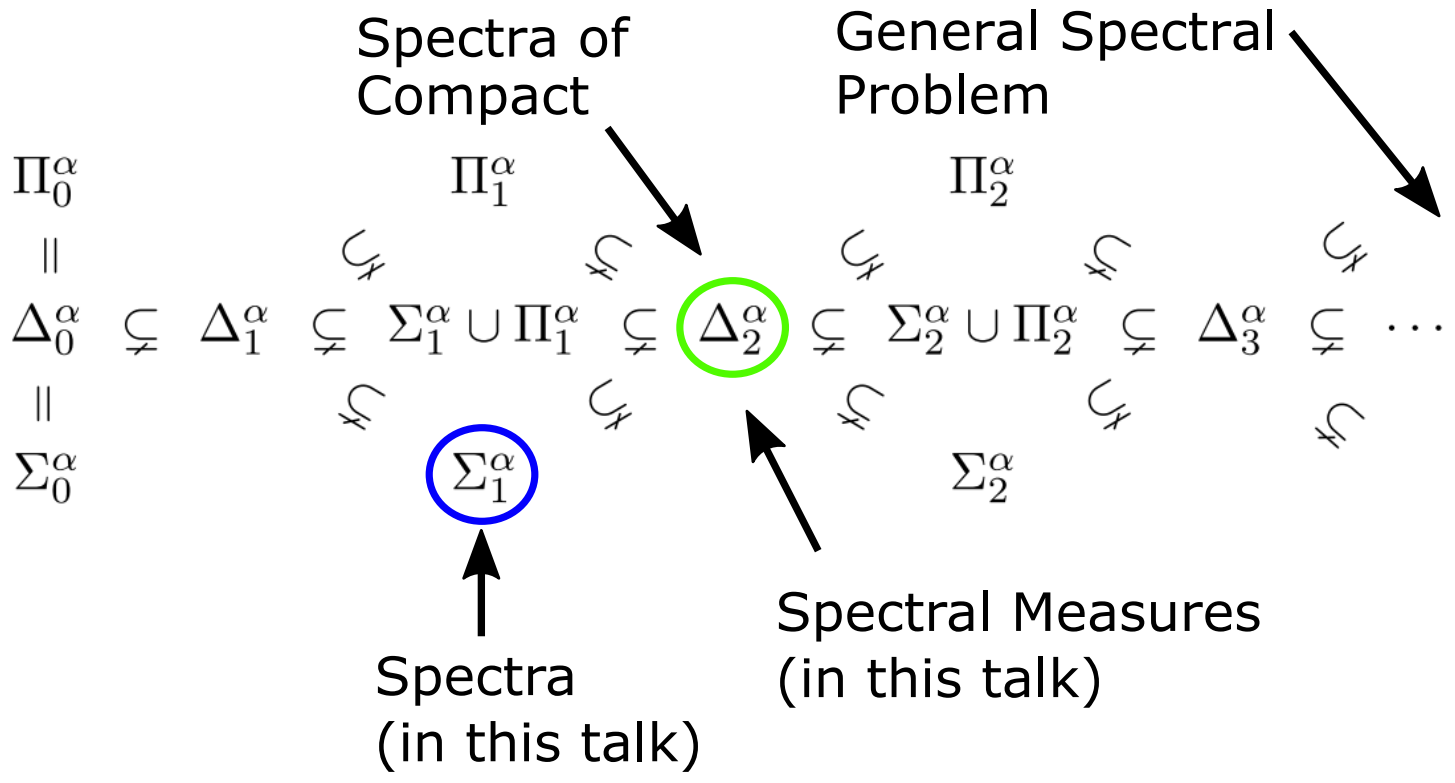
$\Rightarrow$ Algorithms that realise the boundaries of what computers can achieve.

NB: This holds regardless of model of computation - measure the intrinsic difficulty of these problems.

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

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

Structure of the Hierarchy



Example 1: Computing spectra with error control

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

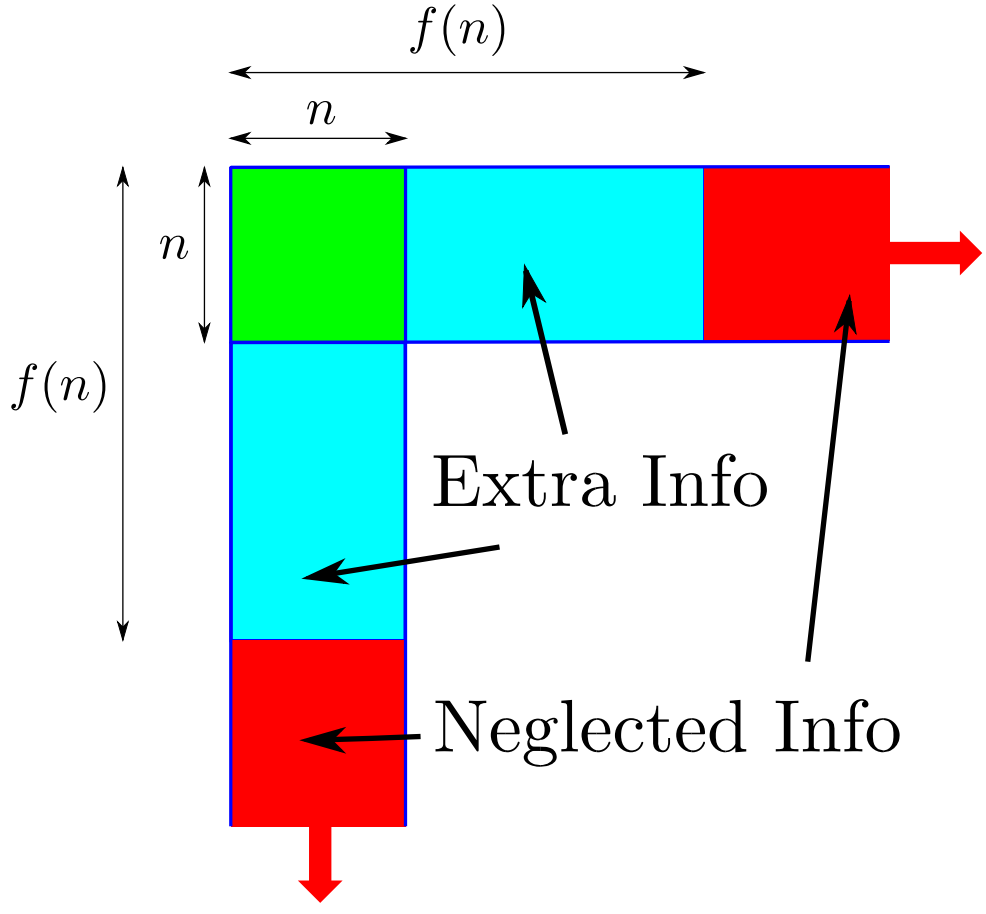
$$\Downarrow$$

First algorithm that computes spectra of a very general class of operators. Also does so with (rigorous provable) error control.

Definition (Dispersion: off-diagonal decay)

Dispersion of A bounded by function $f : \mathbb{N} \to \mathbb{N}$ 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 $g : [0, \infty) \to [0, \infty)$ *with* $g(x) \leq x$.
Controlled growth of the resolvent by g *if*

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

- Measures conditioning of the problem through

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

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

$$\left\|(A - zI)^{-1}\right\|^{-1} = \operatorname{dist}(z, \operatorname{Sp}(A)), \quad g(x) = x.$$

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

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

Step 1: Approximate locally via smallest singular value:

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

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

Step 2: Bound the distance to the spectrum:

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

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

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

NB: Without either f or g, constructing an algorithm convergent to the spectrum is impossible.

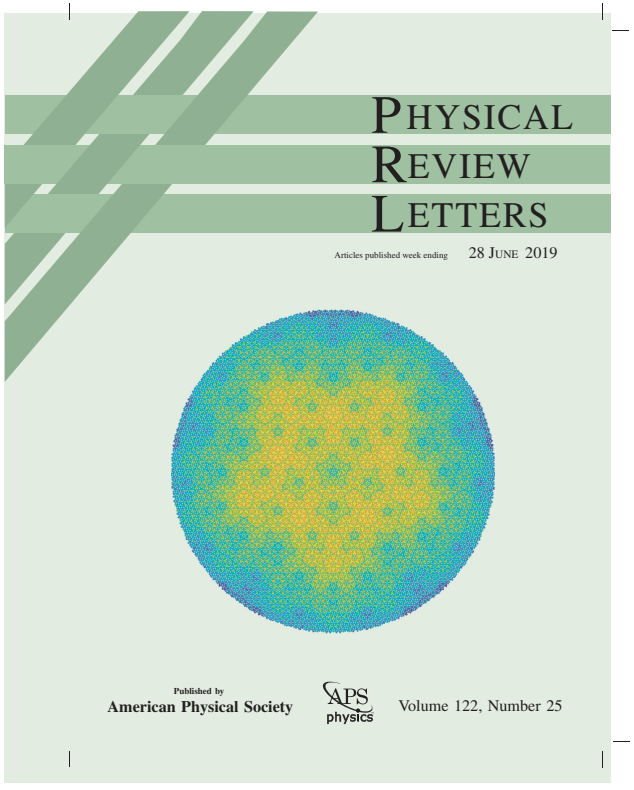
New exemplar of spectral computation

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.



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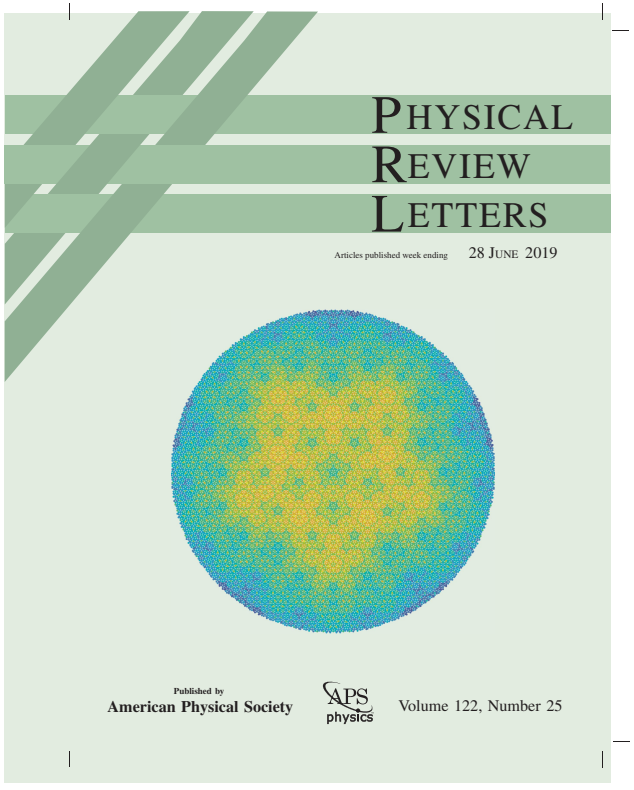


Extends to unbounded operators and PDEs with coefficients of locally bounded total variation (e.g. algorithms point sample coefficients).

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

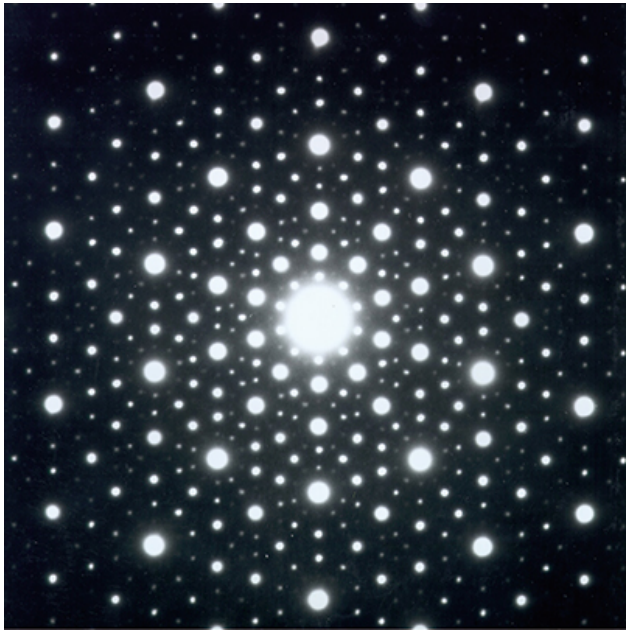


Figure: Left: Dan Shechtman, **Nobel Prize in Chemistry 2011** for discovery of quasicrystal. Right: Diffraction pattern of a quasicrystal.

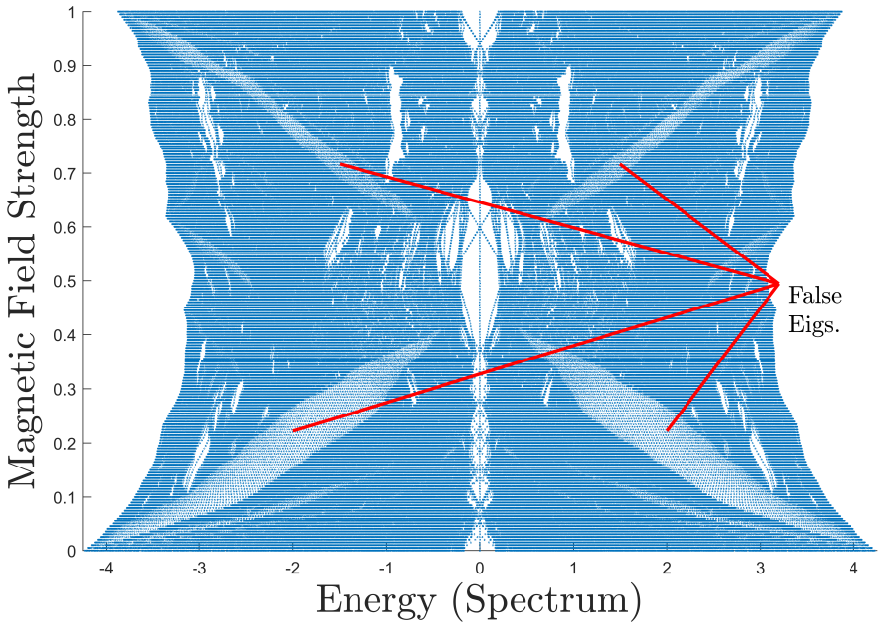
Magnetic properties of quasicrystal.

Hard problem - no previous method even converges to spectrum.

Example: Operators in condensed matter physics

Finite truncations

False 'solutions'.



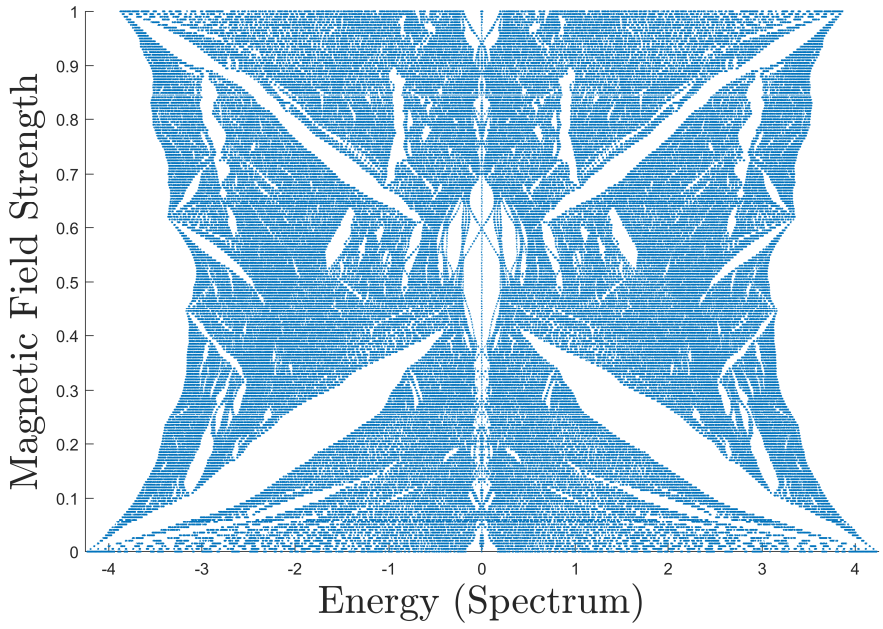
Unreliable

Does not converge

No error control

Infinite-dimensional techniques

First convergent computation.



Reliable

Converges

Error control

Example 2: Computing spectral measures

Computing the action of the resolvent $(A - zI)^{-1}\mathbf{x}$ with asymptotic error control as z approaches $\mathbb{R}$.

$$\Downarrow$$

First algorithm that computes spectral measures (and spectral decompositions) of general self-adjoint operators - 'diagonalisation.'

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

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

Allows computation of functional calculus, has interesting physics etc.

Most previous efforts to develop computational tools have focused on specific examples where analytical formulas are available, or on limit theorems which do not compute the full measure.

Idea: Use the formula

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

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

Smoothed version of measure.

Suppose we compute with a truncation parameter n...

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Theorem (C. Preprint (2019))

Know $f \Rightarrow$ can compute measure in one limit (no error control possible)

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

$$\langle dE * K^\epsilon \mathbf{x}, \mathbf{y}\rangle(x)$$

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

Theorem

Let $n_1 = n_2 = m \in \mathbb{N}$ and fix a_j in UHP, b_j in LHP. Then there exists unique $\{\alpha_j, \beta_j\}$ with the following. For any $\langle dE * K^\epsilon \mathbf{x}, \mathbf{y}\rangle$ absolutely continuous locally around x with C^α Radon–Nikodym derivative F and $\alpha \leq m$, it holds that (up to a possible factor of $\log(\epsilon^{-1})$)

$$|\langle dE * K^\epsilon \mathbf{x}, \mathbf{y}\rangle(x) - F(x)| = \mathcal{O}(\epsilon^\alpha).$$

Example: Jacobi Polynomials

$$d\mu_J = \frac{(1-x)^\alpha (1+x)^\beta}{N(\alpha,\beta)} dx = f_{\alpha,\beta}(x)dx,$$

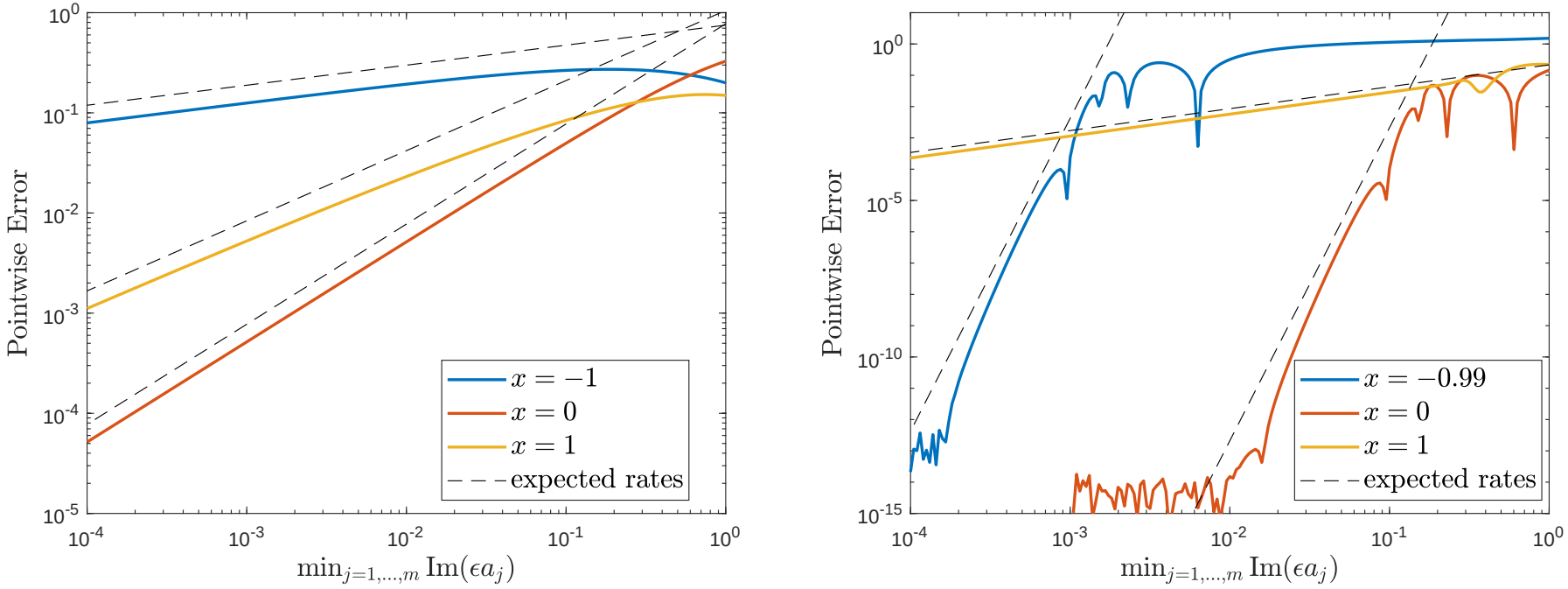

Figure: Left: Pointwise errors for $x = -1, 0, 1$ for $m = 1$ and $\alpha = 0.7$, $\beta = 0.3$. Right: Pointwise errors for $x = -0.99, 0, 1$ for $m = 10$ and $\alpha = 0.7$, $\beta = -0.3$.

Eigenvalue hunting without spectral pollution

Can extend to compute decompositions (of measures and spectral sets).

Example: Dirac operator.

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

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

- Map to $[-1,1]$ using

$$x = \frac{r-L}{r+L}$$

and compute $(A - zI)^{-1}\mathbf{x}$ using the ultraspherical method.

		Abs. Error		
j	$E_{j+1} - E_j$	$n = 10^2$	$n = 10^4$	$n = 10^6$
0	2.94×10^{-1}	1.16×10^{-4}	1.92×10^{-9}	3.08×10^{-14}
1	6.14×10^{-2}	2.23×10^{-5}	3.68×10^{-10}	6.55×10^{-15}
2	2.04×10^{-2}	6.17×10^{-6}	1.01×10^{-10}	1.78×10^{-15}
3	9.02×10^{-3}	2.41×10^{-6}	3.95×10^{-11}	5.55×10^{-16}
4	4.74×10^{-3}	1.17×10^{-6}	1.90×10^{-11}	1.11×10^{-16}
5	2.78×10^{-3}	6.47×10^{-7}	1.05×10^{-11}	1.11×10^{-16}
6	1.77×10^{-3}	3.94×10^{-7}	6.42×10^{-12}	1.11×10^{-16}
7	1.20×10^{-3}	2.57×10^{-7}	4.19×10^{-12}	1.11×10^{-16}
8	8.45×10^{-4}	1.70×10^{-7}	2.88×10^{-12}	2.22×10^{-16}
9	6.18×10^{-4}	8.80×10^{-8}	2.07×10^{-12}	1.11×10^{-16}
10	4.66×10^{-4}	3.68×10^{-8}	1.53×10^{-12}	1.11×10^{-16}
100	6.19×10^{-7}	n/a	2.55×10^{-15}	2.55×10^{-15}
500	5.09×10^{-9}	n/a	n/a	1.11×10^{-12}
1000	6.39×10^{-10}	n/a	n/a	4.00×10^{-13}

NB: This problem is hard! Previous quadratic projection methods compute first four $\{E_0, E_1, E_2, E_3\}$ to at most three digits.

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, ...

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

Coming soon: high-performance numerical package with resolvent based algorithms for discrete and continuous problems (with Andrew Horning).

For papers solving above problems, classifications in the SCI hierarchy and numerical code: http://www.damtp.cam.ac.uk/user/mjc249/home.html