How To Compute Spectra
With Error Control

On The Foundations of Infinite-Dimensional Spectral Computations

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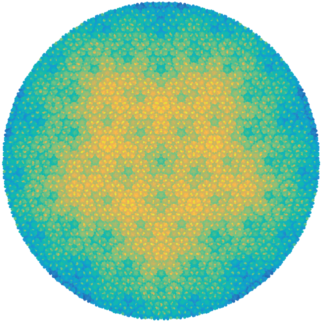
CTAC2020



Main paper:
M.J. Colbrook, B. Roman, and A.C. Hansen
"How to compute spectra with error control"
Physical Review Letters 122.25 (2019)

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

Finite Case		**Infinite Case**
Eigenvalues	$\Rightarrow$	Spectrum $\mathrm{Sp}(A) = \{z \in \mathbb{C} : A - z \text{ not bounded invertible}\}$
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!

Computational spectral problem

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

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),...

However, computing spectra is **notoriously hard**...

London Millennium Bridge:
When computing spectra goes badly wrong!

- Opened on 10 June 2000.
- Spectra correspond to vibrations or “resonances” of bridge.
- Unexpected resonances caused bridge closure on 12 June.
- Closed for two years and cost several million pounds to fix.

Can we do this for general classes of operators?

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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]

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

Turns out this is sharp! Hence impossible from numerical point of view.

[1] Hansen. JAMS (2011)

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Turns out this is sharp! Hence impossible from numerical point of view.
Q: What assumptions do we need to make it easier?

[1] Hansen. JAMS (2011)

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)

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

If $\Gamma_n(A) = \mathrm{Sp}(P_n A P_n)$, then $\Gamma_n(A) \to \mathrm{Sp}(A)$ 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?

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

This problem has been open for decades.

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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!

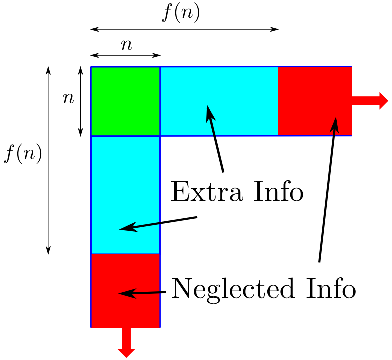
New algorithm (discrete case)

Assume A is bounded and acts on $\ell^2(\mathbb{N})$

Definition (Known 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 (Well-conditioned)

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

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

- Measures conditioning of the problem through

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

- 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* $\mathrm{Sp}(A)$ *with error control!!*

Idea: Locally compute distance function and minimisers

Step 1: Smallest singular value of **rectangular** truncations:

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

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

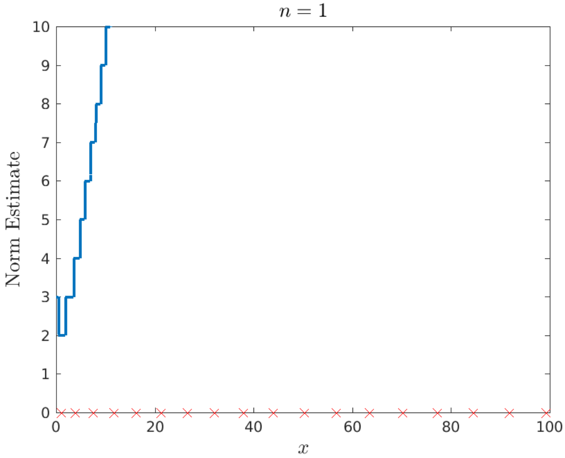
Step 2: Bound the distance to the spectrum:

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

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

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

Example: quartic potential on $L^2(\mathbb{R})$ using a Hermite basis



New exemplar of spectral computation?

Method is:

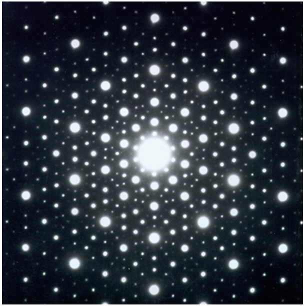
- Local and parallelisable.
- Convergent for first time.
  (e.g. no spectral pollution)
- Explicitly bounds the error:

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

- Optimal from foundations point of view.

Made the frontcover of ***Physical Review Letters***
- American Physical Society's flagship publication

Example: Operators in condensed matter physics



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

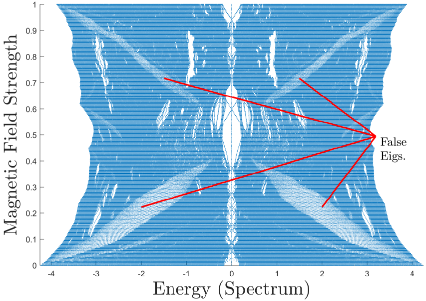
Magnetic properties of quasicrystal.

Hard problem - no previous method even converges to spectrum.

Example: Operators in condensed matter physics

Finite truncations

Edge states.



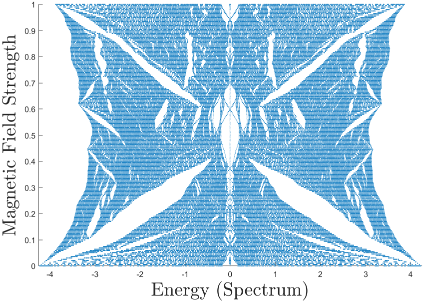
Unreliable

Does not converge

No error control

Infinite-dimensional techniques

First convergent computation.

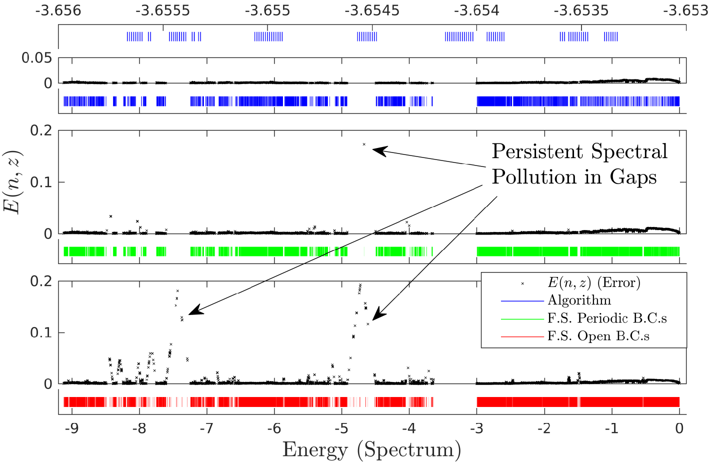


Reliable

Converges

Error control

Example: Laplacian on Penrose tile



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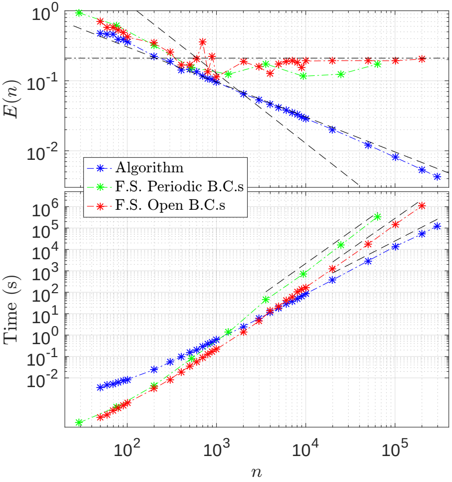


Extension to partial differential operators

Closed operator L on $\mathbb{R}^d$ of form

$$Lu(x) = \sum_{k \in \mathbb{Z}^d_{\geq 0} : |k| \leq N} a_k(x) \partial^k u(x)$$

Assume coefficient functions:

- polynomially bounded
- of bounded total variation on compact balls

($+$ some standard technical assumptions)

$\Rightarrow$ Compute $\mathrm{Sp}(L)$ locally uniformly on compact subsets with error control

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

Executive summary

- Build matrix rep. w.r.t. basis of tensorised Hermite functions.
- Use bound on total variation and quasi-Monte Carlo integration to compute matrix entries of L, L^*L and LL^* with error control.
- Use these estimates to directly approximate $\gamma_n(z)$.
- Apply (roughly) the same algorithm as before.

Details can be found in:
M.J. Colbrook, A.C. Hansen, “The foundations of spectral computations via the Solvability Complexity Index hierarchy: Part I.” arXiv:1908.09592

NB: Can extend technique to other discretisation methods such as FEM.

Example: Eigenvalues with guaranteed error bounds

$$L = -\Delta + x^2 + V(x) \text{ on } L^2(\mathbb{R})$$

V	$\cos(x)$	$\tanh(x)$	$\exp(-x^2)$	$(1+x^2)^{-1}$
E_0	1.7561051579	0.8703478514	1.6882809272	1.7468178026
E_1	3.3447026910	2.9666370800	3.3395578680	3.4757613534
E_2	5.0606547136	4.9825969775	5.2703748823	5.4115076464
E_3	6.8649969390	6.9898951678	7.2225903394	7.3503220313
E_4	8.7353069954	8.9931317537	9.1953373991	9.3168983920

Programme: 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 measuring their intrinsic difficulty and the optimality of algorithms.[2]

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

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 spectra (e.g. capacity), spectral gap problem, spectral measures, ...

[2]Holds regardless of model of computation (Turing, analog,...).

Conclusion

- Can compute spectra of a large class of operators with error control.
- New algorithm is fast, local and parallelisable.
- Methods extend to other problems (e.g. spectral measures) and classify problems into a hierarchy telling us what is possible.

For further details and numerical code:
http://www.damtp.cam.ac.uk/user/mjc249/home.html

Current work:

- Foundations of computational PDEs (e.g. evolution equations)
- Foundations of (stable) computations with neural networks in image reconstruction (new paper on arXiv this month).

References

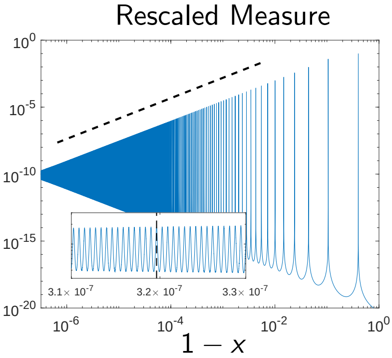
- M.J. Colbrook, B. Roman, and A.C. Hansen. "How to compute spectra with error control." *Physical Review Letters* 122.25 (2019).
- M.J. Colbrook, A.C. Hansen. "On the infinite-dimensional QR algorithm." *Numerische Mathematik* 143.1 (2019).
- M.J. Colbrook, A.C. Hansen. "The foundations of spectral computations via the Solvability Complexity Index hierarchy: Part I." *arXiv preprint*.
- M.J. Colbrook. "The foundations of spectral computations via the Solvability Complexity Index hierarchy: Part II." *arXiv preprint*.
- M.J. Colbrook. "Computing spectral measures and spectral types." *arXiv preprint*.
- M.J. Colbrook, A. Horning, and A. Townsend. "Computing spectral measures of self-adjoint operators." *arXiv preprint*.
- J. Ben–Artzi, M.J. Colbrook, A.C. Hansen, O. Nevanlinna, M. Seidel. "Computing Spectra – On the Solvability Complexity Index Hierarchy and Towers of Algorithms." *arXiv preprint*.

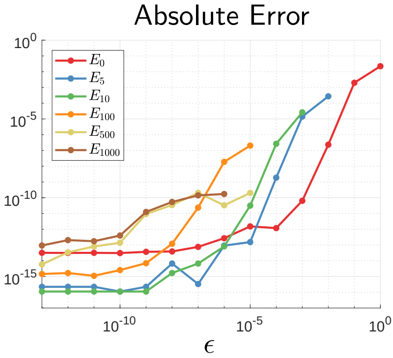
Eigenvalue hunting without spectral pollution

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...

Eigenvalue hunting without spectral pollution





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