On the Solvability Complexity Index hierarchy, the computational spectral problem and computer assisted proofs

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Outline

- Introduction
- Spectral Problems: Infinite Matrices
- Spectral Problems: Schrödinger Operators
- Numerical Examples
- Connections with Logic/Set Theory?
- Computer Assisted Proofs

Motivation

- Motivating example: spectra of infinite-dimensional operators. Many applications but W. Arveson (leading operator theorist U.C. Berkeley) pointed out in the early nineties, "**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.**" Situation was worse for the Schrödinger case!

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- Applications: can we present rigorous computations for the maths/science community and for computer assisted proofs?

Solvability Complexity Index (SCI) [1, Hansen, JAMS]

Ω is some set, called the *primary* set,

Λ is a set of complex valued functions on Ω, called the *evaluation* set,

$\mathcal{M}$ is a metric space, where the thing we compute lives

Ξ is a mapping $\Omega \to \mathcal{M}$, called the *problem* function.

E.g. $\Omega = \mathcal{B}(\mathcal{H})$, problem function Ξ maps $A \mapsto \mathrm{Sp}(A)$, $(\mathcal{M}, d)$ set of all compact subsets of $\mathbb{C}$ with Hausdorff metric and evaluation functions in Λ consist of $f_{i,j} : A \mapsto \langle Ae_j, e_i \rangle$, $i, j \in \mathbb{N}$, which provide the entries of the matrix representation of A w.r.t. an orthonormal basis $\{e_i\}_{i \in \mathbb{N}}$.

Definition 1 (General Algorithm)

Given a computational problem $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$, a *general algorithm* is a mapping $\Gamma : \Omega \to \mathcal{M}$ such that for each $A \in \Omega$:

(i) there exists a finite subset of evaluations $\Lambda_\Gamma(A) \subset \Lambda$,

(ii) the action of Γ on A only depends on $\{A_f\}_{f \in \Lambda_\Gamma(A)}$ where $A_f := f(A)$,

(iii) for every $B \in \Omega$ such that $B_f = A_f$ for every $f \in \Lambda_\Gamma(A)$, it holds that $\Lambda_\Gamma(B) = \Lambda_\Gamma(A)$.

No restrictions on the operations allowed (can consult any fixed oracle etc.). But can consider different types of towers. E.g. type-2 Turing machines, allow radicals, BSS model, ...

Definition 2 (Tower of algorithms)

Given $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$, a *tower of algorithms of height k for* $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$ is a collection of sequences of functions

$$\Gamma_{n_k} : \Omega \to \mathcal{M}, \quad \Gamma_{n_k, n_{k-1}} : \Omega \to \mathcal{M}, \ \ldots \ , \Gamma_{n_k, \ldots, n_1} : \Omega \to \mathcal{M},$$

where $n_k, \ldots, n_1 \in \mathbb{N}$ and the functions $\Gamma_{n_k, \ldots, n_1}$ are general algorithms. Moreover, for every $A \in \Omega$,

$$\lim_{n_k \to \infty} \ldots \lim_{n_1 \to \infty} \Gamma_{n_k, \ldots, n_1}(A) = \Xi(A)$$

with convergence in metric space $\mathcal{M}$.

Definition 3 (Solvability Complexity Index)

$\{\Xi, \Omega, \mathcal{M}, \Lambda\}$ is said to have $\mathrm{SCI}(\Xi, \Omega, \mathcal{M}, \Lambda)_\alpha = k$ with respect to a tower of algorithms of type α if k is the smallest integer for which there exists a tower of algorithms of type α of height k.

If no such tower exists then $\mathrm{SCI}(\Xi, \Omega, \mathcal{M}, \Lambda)_\alpha = \infty$.

If there exists a tower $\{\Gamma_n\}_{n\in\mathbb{N}}$ of type α and height one such that $\Xi = \Gamma_{n_1}$ for some finite n_1, then we define $\mathrm{SCI}(\Xi, \Omega, \mathcal{M}, \Lambda)_\alpha = 0$.

Definition 4 (The Solvability Complexity Index Hierarchy)

Consider a collection $\mathcal{C}$ of computational problems and let $\mathcal{T}$ be the collection of all towers of algorithms of type α for the computational problems in $\mathcal{C}$. Define

$$\Delta_0^\alpha := \{\{\Xi, \Omega\} \in \mathcal{C} \mid \mathrm{SCI}(\Xi, \Omega)_\alpha = 0\}$$

$$\Delta_{m+1}^\alpha := \{\{\Xi, \Omega\} \in \mathcal{C} \mid \mathrm{SCI}(\Xi, \Omega)_\alpha \leq m\}, \qquad m \in \mathbb{N},$$

as well as

$$\Delta_1^\alpha := \{\{\Xi, \Omega\} \in \mathcal{C} \mid \exists \ \{\Gamma_n\}_{n \in \mathbb{N}} \in \mathcal{T} \text{ s.t. } \forall A \ d(\Gamma_n(A), \Xi(A)) \leq 2^{-n}\}.$$

Definition 5 (The SCI Hierarchy (totally ordered set))

Suppose $\mathcal{M}$ is totally ordered. Define

$$\begin{aligned}
&\Sigma_0^\alpha = \Pi_0^\alpha = \Delta_0^\alpha,\\
&\Sigma_1^\alpha = \{\{\Xi,\Omega\} \in \Delta_2 \mid \exists\, \Gamma_n \in \mathcal{T} \text{ s.t. } \Gamma_n(A) \nearrow \Xi(A) \ \ \forall A \in \Omega\},\\
&\Pi_1^\alpha = \{\{\Xi,\Omega\} \in \Delta_2 \mid \exists\, \Gamma_n \in \mathcal{T} \text{ s.t. } \Gamma_n(A) \searrow \Xi(A) \ \ \forall A \in \Omega\},
\end{aligned}$$

where $\nearrow$ and $\searrow$ denotes convergence from below and above respectively, as well as, for $m \in \mathbb{N}$,

$$\begin{aligned}
&\Sigma_{m+1}^\alpha = \{\{\Xi,\Omega\} \in \Delta_{m+2} \mid \exists\, \Gamma_{n_{m+1},\ldots,n_1} \in \mathcal{T} \text{ s.t. } \Gamma_{n_{m+1}}(A) \nearrow \Xi(A) \ \ \forall A \in \Omega\},\\
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\end{aligned}$$

Definition 6 (The SCI Hierarchy (Attouch-Wetts/Hausdorff metric))

Suppose $\mathcal{M}$ is a metric space with the Attouch-Wetts or the Hausdorff metric induced by another metric space $\mathcal{M}'$. Define for $m \in \mathbb{N}$

$$\Sigma_0^\alpha = \Pi_0^\alpha = \Delta_0^\alpha,$$
$$\Sigma_1^\alpha = \{\{\Xi, \Omega\} \in \Delta_2 \mid \exists\ \Gamma_n \in \mathcal{T} \text{ s.t. } \Gamma_n(A) \underset{\mathcal{M}'}{\subset} B_{2^{-n}}^{\mathcal{M}}(\Xi(A)) \ \ \forall A \in \Omega\},$$
$$\Pi_1^\alpha = \{\{\Xi, \Omega\} \in \Delta_2 \mid \exists\ \Gamma_n \in \mathcal{T} \text{ s.t. } B_{2^{-n}}^{\mathcal{M}}(\Gamma_n(A)) \underset{\mathcal{M}'}{\supset} \Xi(A) \ \ \forall A \in \Omega\}.$$

where $\subset_{\mathcal{M}'}$ means inclusion in the metric space $\mathcal{M}'$. Interpret $B_{2^{-n}}^{\mathcal{M}}(x)$ as the subset of $\mathcal{M}'$ given by $\bigcup\{S \subset \mathcal{M}' \mid S \in \mathcal{M}, d_{\mathcal{M}}(S, x) \leq 2^{-n}\}$. Moreover,

$$\Sigma_{m+1}^\alpha = \{\{\Xi, \Omega\} \in \Delta_{m+2} \mid \exists\ \Gamma_{n_{m+1},\ldots,n_1} \in \mathcal{T} \text{ s.t. } \Gamma_{n_{m+1}}(A) \underset{\mathcal{M}'}{\subset} B_{2^{-n}}^{\mathcal{M}}(\Xi(A)) \ \forall A \in \Omega\},$$
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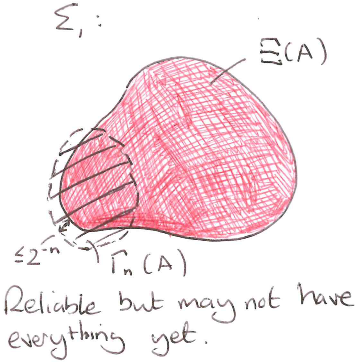
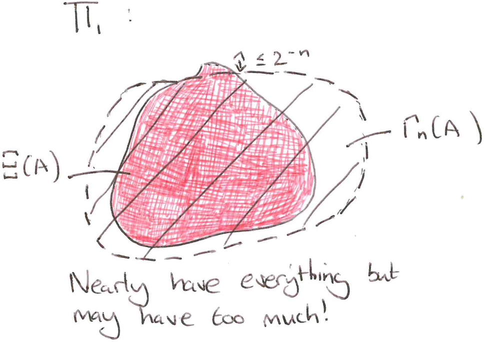
What does this mean?





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- Lower bounds for *general* algorithms provide lower bounds for any reasonable model of computation. But all constructed algorithms can be realised as type-2 Turing machines. Hence results are sharp in this sense - difficulty lies with infinite amount of data/information, not the model of computation.

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- Hence, the field of computational spectral theory is mostly concerned with non-computable problems. Numerical analysts could not solve the spectral problem because they couldn't see the connection with logic.
- Error control for scientific problems - computer assisted proofs?

Computing Spectra with Error Control

- Hilbert space $l^2(\mathbb{N})$ with $\|x\|_2 = \sqrt{\sum_{j=1}^{\infty} |x_j|^2}$, $\langle x, y\rangle = \sum_{j=1}^{\infty} x_j \bar{y}_j$
- Bounded linear operator $A : l^2(\mathbb{N}) \to l^2(\mathbb{N})$ realised as matrix

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

- Want to compute spectrum (generalisation of eigenvalues)

$$\mathrm{Sp}(A) := \{z \in \mathbb{C} : A - zI \text{ not invertible}\}.$$

  from the matrix elements.
- Also the pseudospectrum

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

Two Key Definitions

Definition 7 (Dispersion - off-diagonal decay)

We say that the dispersion of $A \in \mathcal{B}(l^2(\mathbb{N}))$ is bounded by the function $f : \mathbb{N} \to \mathbb{N}$ if

$$D_{f,m}(A) := \max\{\|(I - P_{f(m)})AP_m\|, \|P_m A(I - P_{f(m)})\|\} \to 0 \quad \text{as } m \to \infty.$$

Definition 8 (Controlled growth of the resolvent - well-conditioned)

Let $g : [0, \infty) \to [0, \infty)$ be a continuous function, vanishing only at $x = 0$ and tending to infinity as $x \to \infty$ with $g(x) \leq x$. We say that a closed operator A with non-empty spectrum on the Hilbert space $\mathcal{H}$ has controlled growth of the resolvent by g if

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

where we use the convention $\|B^{-1}\|^{-1} := 0$ if B has no bounded inverse.

What does this mean?

- Dispersion - think banded matrices.
- Controlled resolvent - g is a measure of the conditioning of the problem of computing $\mathrm{Sp}(A)$ through the formula

$$\mathrm{Sp}_\epsilon(A) = \bigcup_{\|B\| \leq \epsilon} \mathrm{Sp}(A + B).$$

- Self-adjoint and normal operators (A commutes with A^*) have well conditioned spectral problems since

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

- Different classes have different classifications in hierarchy...

Example 1: We have both f and g. [2, C. et al.]

- By considering diagonal operators, clear the problem does not lie in Δ_1^G - algorithms can only read a finite amount of information. Hence we wish to show lies in Σ_1^A.

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- Introduce smallest singular value σ_1 (injection modulus) and

$$\gamma(z, A) = \min\{\sigma_1(A - zI), \sigma_1(A^* - \bar{z}I)\} = \|(A - zI)^{-1}\|^{-1},$$
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- Can prove $\gamma_n \downarrow \gamma$ uniformly on compacts.

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- Given f, g and $D_{f,n}(A)$, we can gain an upper bound to $\mathrm{dist}(z, \mathrm{Sp}(A))$ that converges locally uniformly to the true distance. Can use this to build Σ_1^A algorithm.

Example 2: When we have only g, e.g. self-adjoint case.

- How to build Σ_2^A algorithm? Define

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After first limit $n_1 \to \infty$ gain $\gamma_{n_2}(z,A)$ then as before. So only need show this is sharp. I.e. problem does not lie in Δ_2^G.

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- Assume for a contradiction that there is a sequence $\{\Gamma_k\}$ of general algorithms such that $\Gamma_k(A) \to \mathrm{Sp}(A)$ for all $A \in \Omega_{\mathrm{SA}}$, and consider operators of the type

$$A := \bigoplus_{r=1}^{\infty} A_{l_r} \text{ with } \{l_r\} \subset \mathbb{N} \text{ and } A_n := \begin{pmatrix} 1 & & & & 1 \\ & 0 & & & \\ & & \ddots & & \\ & & & 0 & \\ 1 & & & & 1 \end{pmatrix} \in \mathbb{C}^{n \times n}.$$

Simple oscillation argument...

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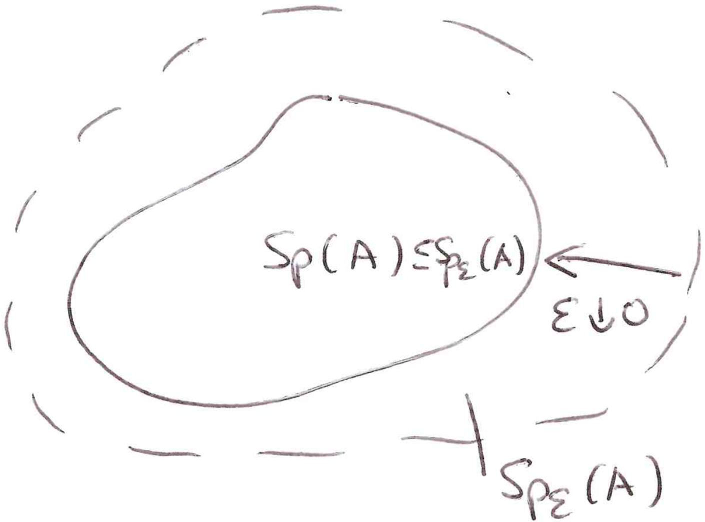
- Without function g (which links Sp and Sp_ϵ), can compute $\mathrm{Sp}_\epsilon(A)$ in two limits. Let $\epsilon = 1/n_3$ then last limit gives convergence from above so Π_3^A.


Sp(A) ⊆ Sp_ε(A)
ε↓0
Sp_ε(A)

Further Results [3]

We have classifications for classes

- Different classes of compact operators
- Normal/self-adjoint/controlled resolvent (g)
- Bounded dispersion
- Diagonal
- General bounded
- Even unbounded
- ...

For problems

- Spectrum
- Pseudospectrum
- Essential Spectrum
- Decision problem: is $z \in \mathrm{Sp}(A)$?
- ...

Schrödinger Operators [3]

- Want to compute spectrum of a Schrödinger operator

$$H = -\Delta + V, \qquad V : \mathbb{R}^d \to \mathbb{C},$$

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- Unsolved for a long time when considering H acting on $\mathrm{L}^2(\mathbb{R}^d)$ allowing non self-adjointness and arbitrary complex potentials.
- Consider the computational problem $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$ with the *Attouch-Wets* metric defined by

$$d_{\mathrm{AW}}(A, B) = \sum_{i=1}^{\infty} 2^{-i} \min\left\{1, \sup_{|x|<i} |d(x, A) - d(x, B)|\right\},$$

  where A and B are closed subsets of $\mathbb{C}$ - generalises Hausdorff distance to general closed sets.

Example: $V \in \mathrm{BV}_\phi(\mathbb{R}^d), \|V\|_\infty \leq M$

- Assume potential in $\mathrm{BV}_\phi(\mathbb{R}^d) = \{f : \mathrm{TV}(f_{[-a,a]^d}) \leq \phi(a)\}$. For simplicity, assume V real-valued.

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- Method: Choose a suitable basis and compute estimations of matrix of operator. Then can use above method (adapted to unbounded closed operators).
- How: Use $V \in \mathrm{BV}_\phi(\mathbb{R}^d), \|V\|_\infty \leq M$ to bound error in integrals from theory of numerical integration.

Generalisations

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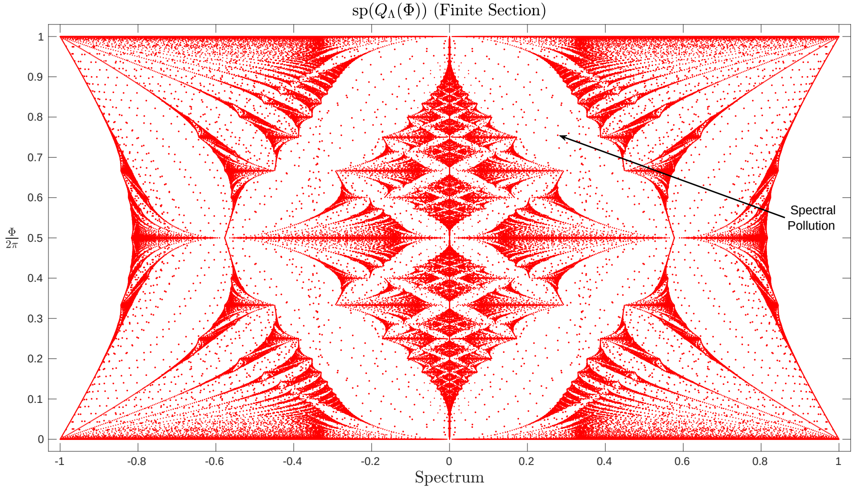
- Can deal with complex potentials also.
- Can build an algorithm for sectorial unbounded potentials with blow up at ∞. Different method - more standard discretisation. Problem lies in Δ_2^A but not $\Sigma_1^G \cup \Pi_1^G$ - same classification as compact operators (realised as infinite matrices).

Graphene


sp($Q_\Lambda(\Phi)$) (Finite Section)
$\frac{\Phi}{2\pi}$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1
Spectrum
Spectral Pollution

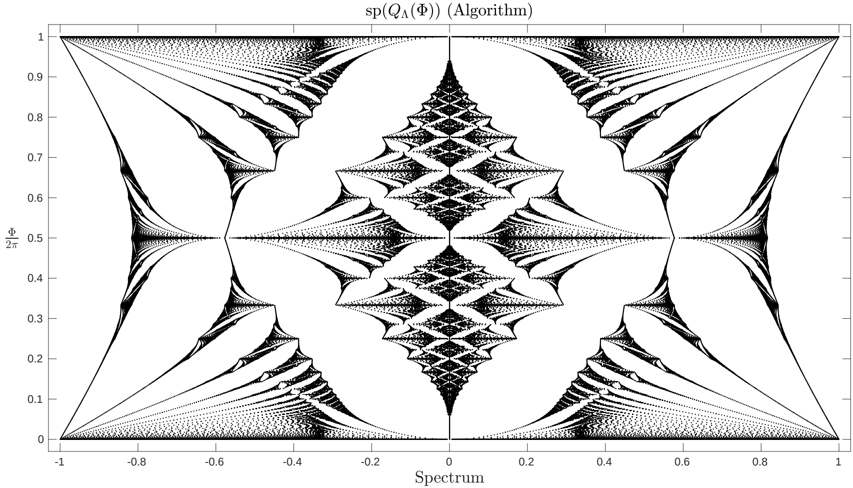
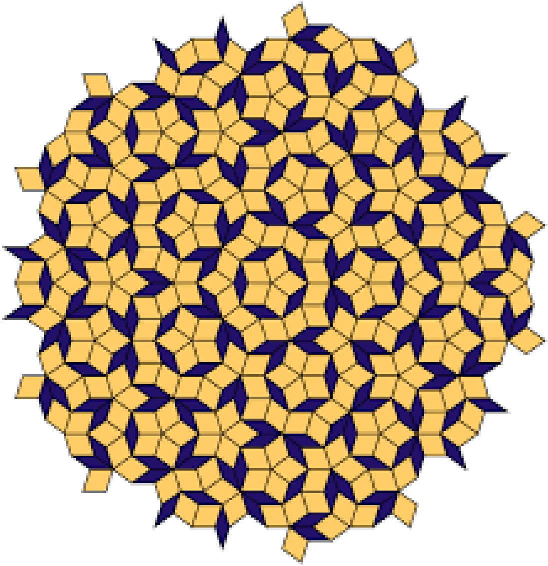
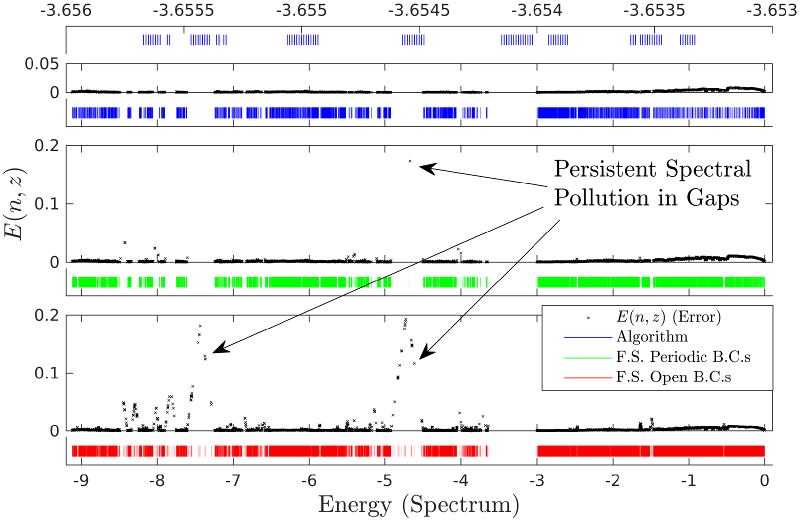


Figure: Guaranteed error bound of 10^{-5}.

Laplacian on Penrose Tile



Laplacian on Penrose Tile



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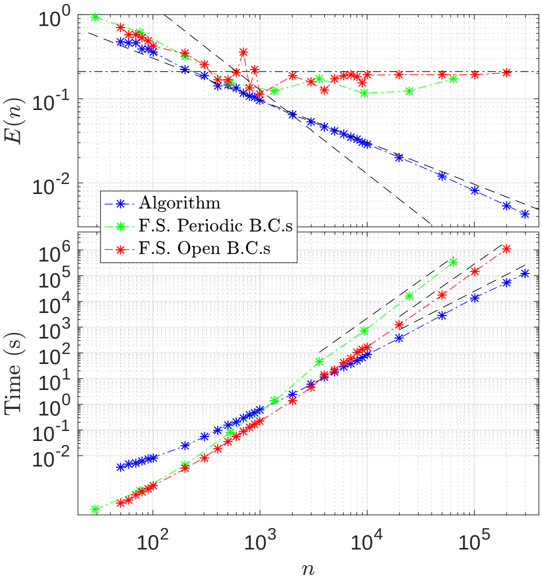

Connections to Logic/Set Theory?

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- However, due to its generality, some of the hierarchies in logic become special cases of the SCI hierarchy.
- As a mathematician with no background in logic, I would be very interested in people's opinions on this and making connections across communities...
- In general, is there a connection with Weihrauch computability? Often its is easier to prove upper bounds without encoding $\mathcal{M}$ but tools developed in this community may be useful for lower bounds. (Again comments and discussion at the end most welcome.)

Very easy example: Arithmetical Hierarchy

Given a subset $A \subset \mathbb{Z}_+$ with characteristic function χ_A definable in First-Order Arithmetic, what is SCI of deciding whether a given number $x \in \mathbb{Z}_+$ belongs to A?

- primary set $\Omega := \mathbb{Z}_+$,
- evaluation set $\Lambda = \{\lambda\}$ consisting of the function $\lambda : \mathbb{Z}_+ \to \mathbb{C}$, $x \mapsto x$,
- metric space $\mathcal{M} := (\{1, 0\}, d_{discr})$.

Definition 9 (Kleene-Shoenfield tower)

A tower of algorithms given by a family $\{\Gamma_{n_k,\dots,n_1} : \Omega \to \mathcal{M} : n_k, \dots, n_1 \in \mathbb{N}\}$ of functions at the lowest level is said to be a *Kleene-Shoenfield tower*, if the function

$$\mathbb{N}^k \times \Omega \to \mathcal{M}, \quad (n_k, \dots, n_1, x) \mapsto \Gamma_{n_k,\dots,n_1}(x)$$

is computable.

Theorem 10 (The SCI hierarchy encompasses the arithmetical hierarchy)

For every $m \in \mathbb{N}$ *we have*

$$\Xi \in \Delta_m \Leftrightarrow \{\Xi, \Omega\} \in \Delta_m^{\mathrm{KS}},$$
$$\Xi \in \Sigma_m \Leftrightarrow \{\Xi, \Omega\} \in \Sigma_m^{\mathrm{KS}},$$
$$\Xi \in \Pi_m \Leftrightarrow \{\Xi, \Omega\} \in \Pi_m^{\mathrm{KS}}.$$

A more interesting result...

Consider $f : \mathbb{R}^* \to \mathbb{R}^*$. A k-tower for f is $F : \mathbb{N}^k \times \mathbb{R}^* \to \mathbb{R}^*$ with

$$f(x_1, \ldots, x_m) = \lim_{n_k \to \infty} \ldots \lim_{n_1 \to \infty} F(n_k, \ldots, n_1, x_1, \ldots, x_m).$$

E. Neumann and A. Pauly recently showed

Theorem 11 ([4])

If $\max\{\mathrm{SCI}_{TTE}(f), \mathrm{SCI}_{BSS}(f)\} \geq 2$ *then* $\mathrm{SCI}_{TTE}(f) = \mathrm{SCI}_{BSS}(f)$.

Since $\mathrm{SCI}_{TTE}(f) \leq n$ iff $f \leq_w \lim^{(n)}$ we obtain that for $n \geq 2$

$$\mathrm{SCI}_{BSS}(f) \geq n \text{ iff } f \not\leq_w \lim^{(n-1)}.$$

So there is some connection with Weihrauch reducibility (for this type of problem function) and a sense of unification for very non-computable problems...

Computer Assisted Proofs

- Recent computer assisted proof of the long lasting Kepler conjecture (Hilbert's 18th problem) is a great example of the use of numerical calculations in a proof [5].

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- Recent computer assisted proof of the long lasting Kepler conjecture (Hilbert's 18th problem) is a great example of the use of numerical calculations in a proof [5].
- The proof relies on deciding more than $50,000$ decision problems in numerical optimisation that are not in Δ_1^G. In particular, the proof hinges on computing undecidable problems.
- Just as most spectral problems of interest are not in Δ_1^G, there are many other crucial problems not in Δ_1^G that may be useful in computer assisted proofs. The key to computer assisted proofs are the classes Σ_1^A and Π_1^A.

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On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators.

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Journal of Complexity, 44:1–22, 2018.

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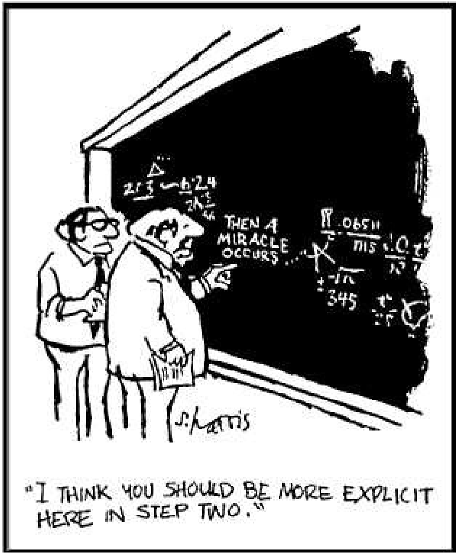
A proof of the Kepler conjecture.

Annals of mathematics, pages 1065–1185, 2005.

Thank you!


THEN A MIRACLE OCCURS
"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."