# 10th Popov Prize: <br> The Solvability Complexity Index Hierarchy 

Matthew J. Colbrook, University of Cambridge FOCM Paris 20/06/2023


## Special thanks to my collaborators!



## Outline

- Solvability Complexity Index Hierarchy and spectral problems.
- Example: Spectra with error control.
- Example: Smale's $18^{\text {th }}$ problem on limits of AI.
- Concluding remarks

Broad goal: classify difficulty of problems, prove optimality of algorithms, figure out what can and cannot be done computationally.

Classical infinite-dimensional spectral problem

$$
\begin{aligned}
& \qquad A "="\left(\begin{array}{ccc}
a_{11} & a_{12} & \cdots \\
a_{21} & a_{22} & \cdots \\
\vdots & \vdots & \ddots
\end{array}\right), \quad A\left(\sum_{k=1}^{\infty} x_{k} e_{k}\right)=\sum_{j=1}^{\infty}\left(\sum_{k=1}^{\infty} a_{j k} x_{k}\right) e_{j} \\
& \text { Also deal with PDEs, integral operators etc. }
\end{aligned}
$$

## Finite-dimensional $\quad \Rightarrow$ Infinite-dimensional

Eigenvalues of $B \in \mathbb{C}^{n \times n} \quad \Rightarrow$ Spectrum, $\operatorname{Sp}(A)$
$\left\{\lambda_{j} \in \mathbb{C}: \operatorname{det}\left(B-\lambda_{j} I\right)=0\right\} \quad \Rightarrow\{\lambda \in \mathbb{C}: A-\lambda I$ is not invertible $\}$

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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. 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)

## What can go wrong?

## Typical approach:

- Matrix case $\left(l^{2}(\mathbb{N})\right)$ : truncate to $\mathcal{P}_{n} A \mathcal{P}_{n}^{*} \in \mathbb{C}^{n \times n}$.
- PDE on unbounded domain: truncate domain then discretise.

Some key issues:
two sources of error

- Spectral pollution (evals accumulate at points not in $\operatorname{Sp}(A)$ as $n \rightarrow \infty$ )
- Spectral invisibility.
- Dealing with essential spectra and continuous spectra.
- Stability, non-normality etc.
- Verification - can we compute spectral properties with error bounds?


## Motivation

- 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, ...
- Specific open problems, e.g., computational quantum mechanics (Schwinger 1960), (Digernes, Varadarajan, Varadhan, 1994):
Given a self-adjoint Schrödinger operator $-\Delta+V$ on $\mathbb{R}$, can we approximate its spectrum from sampling $V$ ?
- Verified computations: Many computer-assisted proofs involve spectra. E.g., $E(Z)=$ ground state energy of $H=\sum_{k=1}^{N}\left(-\Delta_{x_{k}}-Z\left|x_{k}\right|^{-1}\right)+\sum_{j \leq k}\left|x_{j}-x_{k}\right|^{-1}$. Dirac-Schwinger conjecture: asymptotics of $E(Z)$ (Fefferman, Seco 1996)
- Foundations: What is computationally possible? Beyond spectra etc.


# Not all spectral problems are equally hard ... 

## Warm-up: bounded diagonal operators

$$
A=\left(\begin{array}{lll}
a_{1} & & \\
& a_{2} & \\
& & \ddots
\end{array}\right)
$$

Assumption: Algorithm can query entries of $A$
Algorithm: $\Gamma_{n}(A)=\left\{a_{1}, a_{2}, \ldots, a_{n}\right\} \rightarrow \operatorname{Sp}(A)=\overline{\left\{a_{1}, a_{2}, \ldots\right\}}$ in Haus. Metric.
One-sided error control: $\Gamma_{n}(A) \subset \operatorname{Sp}(A)$

$$
d_{\mathrm{H}}(X, Y)=\max \left\{\sup _{x \in X} d(x, Y), \sup _{y \in Y} d(y, X)\right\}
$$

Optimal: Can't obtain $\hat{\Gamma}_{n}(A) \rightarrow \operatorname{Sp}(A)$ with $\operatorname{Sp}(A) \subset \hat{\Gamma}_{n}(A)$.

## Warm-up: compact self-adjoint operators



$$
A=\left(\begin{array}{ccc}
a_{11} & a_{12} & \cdots \\
a_{21} & a_{22} & \cdots \\
\vdots & \vdots & \ddots
\end{array}\right)
$$

Algorithm: $\Gamma_{n}(A)=\operatorname{Sp}\left(\mathcal{P}_{n} A \mathcal{P}_{n}^{*}\right)$ converges to $\operatorname{Sp}(A)$ in Haus. Metric. Question: Can we verify the output?
i.e., Does there exist some alg. $\hat{\Gamma}_{n}(A) \rightarrow \operatorname{Sp}(A)$ with $\hat{\Gamma}_{n}(A) \subset \operatorname{Sp}(A)+B_{2}-n$ ?

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i.e., Does there exist some alg. $\hat{\Gamma}_{n}(A) \rightarrow \operatorname{Sp}(A)$ with $\hat{\Gamma}_{n}(A) \subset \operatorname{Sp}(A)+B_{2^{-n}}$ ?

Answer: No algorithm can do this on whole class!

## What about Jacobi operators?

$$
A=\left(\begin{array}{cccc}
a_{1} & b_{1} & & \\
b_{1} & a_{2} & b_{2} & \\
& b_{2} & a_{3} & \ddots \\
& & \ddots & \ddots
\end{array}\right), \quad b_{k}>0, \quad a_{k} \in \mathbb{R}
$$

Non-trivial, e.g., spurious eigenvalues.

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Sparse: finitely many non-zeros in each column
Non-trivial, e.g., spurious eigenvalues. Enlarge class to sparse normal operators - surely now much harder?! Answer: $\exists\left\{\Gamma_{n}\right\}$ s.t. $\lim _{n \rightarrow \infty} \Gamma_{n}(A)=\operatorname{Sp}(A)$ and $\Gamma_{n}(A) \subset \operatorname{Sp}(A)+B_{2^{-n}}$, for any sparse normal operator $A$

## A curious case of limits

General bounded: $\quad A=\left(\begin{array}{ccc}a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots\end{array}\right)$

$$
\text { Algorithm: } \exists\left\{\Gamma_{n_{3}, n_{2}, n_{1}}\right\} \text { s.t. } \lim _{n_{3} \rightarrow \infty} \lim _{n_{2} \rightarrow \infty} \lim _{n_{1} \rightarrow \infty} \Gamma_{n_{3}, n_{2}, n_{1}}(A)=\operatorname{Sp}(A)
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Question: Can we do better?

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General bounded:

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Question: Can we do better?
Answer: No! Canonically embed problems such as:

## Explains Arveson's lament!

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 (indep. of comp. model).

## General algorithm: beyond recursion theory

Computational problem:

- Class of objects $\Omega$ (e.g., operators).
- Metric space ( $\mathcal{M}, d$ ) (e.g., Hausdorff metric).
- Thing we want to compute $\Xi: \Omega \rightarrow \mathcal{M}$.
- Info we can access, $\Lambda$ a set of functions $\Omega \rightarrow \mathbb{C}$ (e.g., matrix entries).

General algorithm: map $\Gamma: \Omega \rightarrow \mathcal{M}$ such that for any $A \in \Omega, \exists$ a finite non-empty subset $\Lambda_{\Gamma}(A) \subseteq \Lambda$ such that

$$
B \in \Omega, f(B)=f(A) \forall f \in \Lambda_{\Gamma}(A) \Rightarrow \Lambda_{\Gamma}(A)=\Lambda_{\Gamma}(B), \Gamma(A)=\Gamma(B)
$$

A lower bound for general algorithms holds in ALL models of computation.

## Solvability Complexity Index Hierarchy

- $\Delta_{0}$ : Solved in finite time ( v . rare for cts problems).
- $\Delta_{1}$ : Solved in "one limit" with full error control:

$$
d\left(\Gamma_{n}(A), \Xi(A)\right) \leq 2^{-n}
$$

- $\Delta_{2}$ : Solved in "one limit":

$$
\lim _{n \rightarrow \infty} \Gamma_{n}(A)=\Xi(A)
$$

- $\Delta_{3}$ : Solved in "two successive limits":

$$
\vdots \quad \lim _{n \rightarrow \infty} \lim _{m \rightarrow \infty} \Gamma_{n, m}(A)=\Xi(A)
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Can work in any model. E.g., BSS machine, Turing machine, interval arithmetic, inexact input etc.

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Steve Smale: "Is there any purely [rational] iterative generally convergent algorithm for polynomial zero finding?"

Curt McMullen: "Yes, if the degree is three; no, if the degree is higher."

Peter Doyle \& Curt McMullen: "The problem can be solved using successive limits for the quartic and quintic, but not the sextic."

Can work in any model. E.g., BSS machine, Turing machine, interval arithmetic, inexact input etc.

- 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.

## Error control for spectral problems

$$
d_{\mathrm{H}}(X, Y)=\max \left\{\sup _{x \in X} d(x, Y), \sup _{y \in Y} d(y, X)\right\}
$$

$\Sigma_{1}$ convergence


- $\Sigma_{1}: \exists$ alg. $\left\{\Gamma_{n}\right\}$ s.t. $\lim _{n \rightarrow \infty} \Gamma_{n}(A)=\Xi(A), \max _{z \in \Gamma_{n}(A)} \operatorname{dist}(z, \Xi(A)) \leq 2^{-n}$


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$$

$\Sigma_{1}$ convergence
$\Pi_{1}$ convergence

$$
\Xi(A)=\operatorname{Sp}(A)
$$



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$\cdot \Pi_{1}: \exists$ alg. $\left\{\Gamma_{n}\right\}$ s.t. $\lim _{n \rightarrow \infty} \Gamma_{n}(A)=\Xi(A), \max _{z \in \Xi(A)} \operatorname{dist}\left(z, \Gamma_{n}(A)\right) \leq 2^{-n}$

[^0]Sampler of results for bounded op. on $l^{2}(\mathbb{N})$


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# Sampler of results for bounded op. on $l^{2}(\mathbb{N})$ 

increasing difficulty


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.
- C.', "On the computation of geometric features of spectra of linear operators on Hilbert spaces," Found. Comput. Math., 2022.
- C., Hansen, "The foundations of spectral computations via the solvability complexity index hierarchy," J. Eur. Math. Soc., 2023.
- C., "Computing spectral measures and spectral types," Commun. Math. Phys., 2021.
- C., Horning, Townsend, "Computing spectral measures of self-adjoint operators," SIAM Rev., 2021.
- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," preprint.


## Example 1: $\Sigma_{1}$ algorithm for spectra

$\Sigma_{1}$ convergence


## Two reasons its hard!

$$
\begin{aligned}
& A=\oplus_{r=1}^{\infty} J_{l_{r}}, \quad J_{l_{r}}=\left(\begin{array}{cccc}
0 & 1 & & \\
& 0 & \ddots & \\
& & \ddots & 1 \\
& & & 0
\end{array}\right) \in \mathbb{C}^{l_{r} \times l_{r}} \\
& \operatorname{Sp}(A)= \begin{cases}\{0\}, & \text { sup } l_{r}<\infty \\
\{z:|z| \leq 1\}, & \text { otherwise }\end{cases}
\end{aligned}
$$

Instability

No algorithm when given $\left\{l_{r}\right\}_{r=1}^{\infty}$ can determine if it is bounded. $\Rightarrow$ No algorithm computes spectra of gen. tridiagonal operators.

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> Always have:
> $\left\|(A-z)^{-1}\right\|^{-1} \leq \operatorname{dist}(z, \operatorname{Sp}(A))$

## Assume:

known function

$$
g(\operatorname{dist}(z, \operatorname{Sp}(A))) \leq\left\|(A-z)^{-1}\right\|^{-1}
$$

## Two reasons its hard!

$$
\begin{aligned}
& A=\oplus_{r=1}^{\infty} A_{l_{r}}, \quad A_{l_{r}}=\left(\begin{array}{ccccc}
1 & & & & 1 \\
& 0 & & & \\
& & \ddots & 0 & \\
1 & & & & 1
\end{array}\right) \in \mathbb{C}^{l_{r} \times l_{r}} \\
& \operatorname{Sp}(A)=\{0,2\}, \quad \operatorname{Sp}(\operatorname{diag}(1,0, \ldots))=\{0,1\}
\end{aligned}
$$

More involved: choose $\left\{l_{r}\right\}_{r=1}^{\infty}$ to trick any supposed algorithm (try it!)

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\begin{aligned}
& A=\oplus_{r=1}^{\infty} A_{l_{r}}, \quad A_{l_{r}}=\left(\begin{array}{ccccc}
1 & & & & 1 \\
& 0 & & & \\
& & \ddots & & \\
1 & & & 0 & \\
\text { Info at } \infty
\end{array}\right) \in \mathbb{C}^{l_{r} \times l_{r}} \\
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## Assume:

We have access $(\Lambda)$ to inner products

$$
\left\langle A e_{j}, e_{i}\right\rangle, \quad\left\langle A e_{j}, A e_{i}\right\rangle, \quad\left\langle A^{*} e_{j}, A^{*} e_{i}\right\rangle
$$

# Sketch of method 

Spectra through
injection moduli (smallest singular value)
$\mathcal{P}_{n}=$ orthog-projection onto span\{ $\left\{e_{1}, \ldots, e_{n}\right\}$

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

$$
\begin{array}{r}
\left\|(A-z)^{-1}\right\|^{-1}=\min \left\{\sigma_{\mathrm{inf}}(A-z), \sigma_{\mathrm{inf}}\left(A^{*}-\bar{z}\right)\right\} \\
\sqrt{\sigma_{\mathrm{inf}}\left(\mathcal{P}_{n}(A-z)^{*}(A-z) \mathcal{P}_{n}^{*}\right)}=\sigma_{\mathrm{inf}}\left([A-z] \mathcal{P}_{n}^{*}\right) \downarrow \sigma_{\mathrm{inf}}(A-z) \\
g^{-1}\left(\sqrt{\sigma_{\mathrm{inf}}\left(\mathcal{P}_{n}[A-z]^{*}[A-z] \mathcal{P}_{n}^{*}\right)}\right) \downarrow g^{-1}\left(\left\|(A-z)^{-1}\right\|^{-1}\right) \geq \operatorname{dist}(z, \operatorname{Sp}(A)) \\
\left\|(A-z)^{-1}\right\|^{-1} \geq g(\operatorname{dist}(z, \operatorname{Sp}(A)))
\end{array}
$$

Error control!
Final ingredient: adaptive search for local minimisers.

## What did we do?

> See conditions to make possible!

- Lower bound: embed a problem of known difficulty.

Now have canonical ways to do this.
Holds regardless of computational model.

- Upper bound: build an algorithm.

Problem dependent.
Often, infinite-dimensional solve-then-discretise needed

Typically involves resolvent $(A-z)^{-1}$ for spectral problems.

NB: One can show without $g$ or $\left\langle A e_{j}, A e_{i}\right\rangle,\left\langle A^{*} e_{j}, A^{*} e_{i}\right\rangle, \mathrm{SCI} \geq 2$.

## Example: Quasicrystal





Dan Shechtman (Nobel Prize in Chemistry 2011.)



Carl Bender


Michael Berry

## Example with non-trivial $g$

$$
\left\|(T-z)^{-1}\right\|^{-1}
$$

$$
T=-\frac{d^{2}}{d x^{2}}+i x^{3} \text { on } \mathbb{R}
$$

$j \quad E_{j}$ to 30 digits with int. arith.

$1 \quad 1.1562670719881132937992191779999$ 4.1092287528096515358436684785613 7.5622738549788280413518091106314 11.3144218201958044022337839484269 15.2915537503925323881816307917519 19.4515291306917283146861117141044 23.7667404354858191315580259687899 28.2175249729811932975950538782689 $9 \quad 32.7890827818629574924473714850463$ $10 \quad 37.4698253605160468664288735945305$ 100627.6947122484365113526737029011536

## Differential operators on $L^{2}\left(\mathbb{R}^{d}\right)$

Theorem: $\Omega$ : class of self-adjoint diff. operators on $L^{2}\left(\mathbb{R}^{d}\right)$

$$
T=\sum_{k \in \mathbb{Z}_{\geq 0}^{d},|k| \leq N} c_{k}(x) \partial^{k}
$$

- $C_{0}^{\infty}\left(\mathbb{R}^{d}\right)$ a core of $T$.
- $\left\{c_{k}\right\}$ poly bounded, locally bounded total variation.

Can access (to arbitrary precision):

- $\left\{c_{k}(q)\right\}$ for $q \in \mathbb{Q}^{d}$.
- Polynomial that bounds $\left\{c_{k}\right\}$ on $\mathbb{R}^{d}$.
(a) Know $\left\|c_{k}\right\|_{\mathrm{TV}\left([-n, n]^{d}\right)} \leq b_{n} \Rightarrow\{\mathrm{Sp}, \Omega\} \in \Sigma_{1}$.
(b) Know $\left\|c_{k}\right\|_{\mathrm{TV}\left([-n, n]^{d}\right)}=O\left(b_{n}\right) \Rightarrow\{\mathrm{Sp}, \Omega\} \in \Delta_{2} \backslash\left(\Sigma_{1} \cup \Pi_{1}\right)$.


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Sampling schemes
to construct matrix.

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(a) Know $\left\|c_{k}\right\|_{\mathrm{TV}\left([-n, n]^{d}\right)} \leq b_{n} \Longrightarrow\{\mathrm{Sp}, \Omega\} \in \Sigma_{1}$.

Verifiable
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## Not verifiable

## Example 2: Smale's 18th problem "What are the limits of Al?"

"Very often, the creation of a technological artifact precedes the science that goes with it. The steam engine was invented before thermodynamics. Thermodynamics was invented to explain the steam engine, essentially the limitations of it. What we are after is the equivalent of thermodynamics for intelligence." Yann LeCun

## Lower bounds: Use SCI embedding techniques

randomized sequential general algorithms $-\cdots$<br>capture adaptive and probabilistic choice of training data

## Problem: hallucinations and instability

"AI hallucination", from Facebook and NYU’s FastMRI challenge 2020.
Original image AI reconstruction

"Such hallucinatory features are not acceptable and especially problematic if they mimic normal structures that are either not present or actually abnormal."

Instabilities in medical diagnosis Original Mole

Perturbed Mole


Model confidence
$\square$ Benign
Malignant
Model confidence
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 exists, but it can never be trained!
E.g., suppose we want to solve (holds for much more general problems)

$$
\min _{x \in \mathbb{C}^{N}}\|x\|_{l^{1}}+\lambda\|A x-y\|_{l_{2}}^{2}
$$

$$
A \in \mathbb{C}^{m \times N}(\text { modality }, m<N), \quad S=\left\{y_{K}\right\}_{K=1}^{R} \text { (samples) }
$$

Arises when given $y \approx A x+e$.
Enforce condition numbers bounded by 1 .

## Input data $\Lambda$

$$
A \in \mathbb{C}^{m \times N} \text { (modality, } m<N \text { ), } \quad S=\left\{y_{k}\right\}_{k=1}^{R} \text { (samples) }
$$

In practice, $A$ not known exactly or stored to finite precision.
Assume access to $\left\{y_{n, k}\right\}_{k=1}^{R}$ and $A_{n}$ (rational approx, e.g., floats) such that

$$
\left\|y_{n, k}-y_{k}\right\| \leq 2^{-n}, \quad\left\|A_{n}-A\right\| \leq 2^{-n}, \quad n \in \mathbb{N}
$$

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

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

In a nutshell: allow access to arbitrary precision training data.
Question: Given a collection $\Omega$ of $(A, S)$, does there exist a neural network approximating the solution map, and can it be trained by an algorithm?

## What could go wrong?

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Question: Given a collection $\Omega$ of $(A, S)$, does there exist a neural network approximating the solution map, and can it be trained by an algorithm?

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1. Non-existence: No neural network approximates solution map $\Xi$.

## What could go wrong?

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\min _{x \in \mathbb{C}^{N}}\|x\|_{l^{1}}+\lambda\|A x-y\|_{l_{2}}^{2}
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What could go wrong?

## 1. Non-existence: No neural network approximates solution map $\bar{g}$.

2. Non-trainable: $\exists$ neural network that approximates $\Xi$, but it can't be trained.
3. Not practical: $\exists$ neural network that approximates $\Xi$, and training algorithm. However, any training algorithm needs prohibitively many samples.

## Fundamental barriers

Paradox: "Nice" linear inverse problems where a stable and accurate neural network for image reconstruction exists, but it can never be trained!

Theorem: Pick positive integers $n \geq 3$ and $M$. Class of problems such that:

- (Not trainable) No algorithm (even random) can train a neural network with $\boldsymbol{n}$ digits of accuracy over dataset with prob. $>1 / 2$.
- (Not practical) $\boldsymbol{n}-\mathbf{1}$ digits of accuracy possible over dataset, but any training algorithm requires arbitrarily large training data.
- (Trainable and practical) $\boldsymbol{n} \mathbf{- 2}$ digits of accuracy possible over dataset via training algorithm using $\boldsymbol{M}$ training data.

Holds for any architecture, any precision of training data.
$\Rightarrow$ Classification theory telling us what can and cannot be done

[^1]Low-dimensional phase transitions


## Idea of mechanism

SCl embedding into well-conditioned problems.


Randomised general algorithm to capture training.


Workhorse lemma (applies to other problems).

## 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: stable neural networks trained with exponential accuracy. E.g., approximate sharpness inequality:

$$
\begin{gathered}
\min _{x \in \mathbb{C}^{N}} f(x) \quad \text { s.t. } \quad\|A x-y\| \leq \varepsilon \\
\operatorname{dist}\left(x, \text { solution set) } \leq\left(\frac{\left(\left[f(x)-f^{*}\right]+[\|A x-y\|-\varepsilon]+\delta\right.}{\alpha}\right)^{1 / \beta}\right. \\
\begin{array}{c}
\text { Fast Iterative REstarted NETworks (FIRENETs) } \\
\text { (unrolled primal-dual with novel restart scheme) }
\end{array}
\end{gathered}
$$

Theorem: Training algorithm under above assumption produces stable neural networks $\varphi_{n}$ of width $O(N)$, depth $O(n)$, guaranteed worst bound optimal in $(\alpha, \beta)$. E.g., $\beta=1$,

$$
\operatorname{dist}\left(\varphi_{n}(y), \text { solution set }\right) \lesssim e^{-n}+\delta
$$

## Example of severe instability

Original $x$
$x+e_{1}$
$x+e_{2}$
$x+e_{3}$

$\Psi\left(A\left(x+e_{1}\right)\right)$
$\Psi\left(A\left(x+e_{2}\right)\right)$


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


## Stability vs accuracy



Original (cropped, red frame)


Original + detail $\left(x+h_{1}\right)$ (cropped, blue frame)


## U-Net with no noise: accurate but unstable

Original $x$
(full size)


Original


Original + detail $\left(x+h_{1}\right)$ (cropped, blue frame)



Original $x$


Original
(cropped, red frame)

Original + detail $\left(x+h_{1}\right)$ (cropped, blue frame)


FIRENET: balances stability and accuracy?

Original $x$
(full size)

Original (cropped, red frame)

Original + detail $\left(x+h_{1}\right)$ (cropped, blue frame)


FIRENET: balances stability and accuracy?

Original $x$


Original
(cropped, red frame)

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Open problem: use the toolkit to discover optimal trade-offs.

## Why study this hierarchy?

- Optimality: understand boundaries of what's possible.
- Lower bounds $\Rightarrow$ spot assumptions needed to lower SCI.
- Upper bounds $\Rightarrow$ new algorithms and methods.


## FOUNDATIONS $\longleftrightarrow$ METHODS

- $\Sigma_{1} \cup \Pi_{1} \Rightarrow$ computer-assisted proofs.
- Much of computational literature not sharp!


## Remarks:

- Can use any model of computation.
- Existing hierarchies (e.g., arithmetic, Baire etc.) included as particular cases.


## SCI throughout computational mathematics

- Resonances $\left(\Delta_{2} \backslash \Sigma_{1} \cup \Pi_{1}\right)$
- Ben-Artzi, Marletta, Rösler, "Computing scattering resonances," J. Eur. Math. Soc., 2022.
- Ben-Artzi, Marletta, Rösler, "Computing the sound of the sea in a seashell," Found. Comput. Math., 2022.
- Optimisation and regularisation
- Bastounis, Hansen, Vlačić, "The extended Smale's 9th problem," preprint.
- C., Gazdag, Bastounis, Hansen, "On phase transitions and approximation thresholds in semidefinite programs," preprint.
- Data-driven Koopmanism for dynamical systems (40,000 papers 2013-2023)
- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," CPAM, to appear.
- C., Ayton, Szőke, "Residual Dynamic Mode Decomposition," J. Fluid Mech., 2023.
- Polynomial root finding $\left(\Delta_{2}, \Delta_{3}, \Delta_{4}\right)$
- Smale, "The fundamental theorem of algebra and complexity theory," Bull. Amer. Math. Soc., 1981.
- McMullen, "Families of rational maps and iterative root-finding algorithms," Ann. of Math., 1987.
- Doyle, McMullen, "Solving the quintic by iteration," Acta Math., 1989.


## SCI throughout computational mathematics

- Computer-assisted proofs ( $\Sigma_{1} \cup \Pi_{1} \backslash \Delta_{1}$ )
- Fefferman, Seco, "Aperiodicity of the Hamiltonian flow in the Thomas-Fermi potential," Rev. Mat. Iberoamericana, 1993.
- Fefferman, Seco, "Interval arithmetic in quantum mechanics," Applications of interval computations, 1996.
- 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.
- Spectral measures and continuous spectra ( $\Delta_{1}$ or $\Delta_{2}$ depending on $(\mathcal{M}, d)$ )
- Webb, Olver, "Spectra of Jacobi operators via connection coefficient matrices," CIMP, 2021.
- C., Horning, Townsend, "Computing spectral measures of self-adjoint operators," SIAM Rev., 2021.


Andrew Horning delivering plenary on computing spectral measures at SIAMCSE23

## Summary

SCI hierarchy is a tool for discovering the foundations of computation.
Example 1: The zoo of spectral problems.

- Many spectral problems in infinite dimensions are impossible. Some are more impossible than others!
- New suite of "infinite-dimensional" algorithms for spectral problems. Rigorous, optimal, practical.
Example 2: Need for foundations in AI/deep learning (Smale's $18^{\text {th }}$ prob).
- Paradox: "Nice" problems where stable, accurate NNs exist but can't be trained! Trainability depends on desired accuracy, training data.
- Conditions $\Rightarrow$ FIRENETs exp. convergence + stable (even w.r.t. adversarial attacks).


## Could this framework be useful in your area?

## References

[1] Colbrook, Matthew J., Vegard Antun, and Anders C. Hansen. "The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem." Proceedings of the National Academy of Sciences 119.12 (2022): e2107151119. [2] Antun, V., M. J. Colbrook, and A. C. Hansen. "Proving existence is not enough: Mathematical paradoxes unravel the limits of neural networks in artificial intelligence." SIAM News 55.4 (2022): 1-4.
[3] Colbrook, Matthew, Vegard Antun, and Anders Hansen. "Mathematical paradoxes unearth the boundaries of AI." TheScienceBreaker 8.3 (2022).
[4] Adcock, Ben, Matthew J. Colbrook, and Maksym Neyra-Nesterenko. "Restarts subject to approximate sharpness: A parameter-free and optimal scheme for first-order methods." arXiv preprint arXiv:2301.02268 (2023).
[5] Colbrook, Matthew J. "WARPd: A linearly convergent first-order primal-dual algorithm for inverse problems with approximate sharpness conditions." SIAM Journal on Imaging Sciences 15.3 (2022): 1539-1575. [6] Colbrook, Matthew. The foundations of infinite-dimensional spectral computations. Diss. University of Cambridge, 2020.
[7] Ben-Artzi, J., Colbrook, M. J., Hansen, A. C., Nevanlinna, O., \& Seidel, M. (2020). Computing Spectra--On the Solvability Complexity Index Hierarchy and Towers of Algorithms. arXiv preprint arXiv:1508.03280.
[8] Colbrook, Matthew J., and Anders C. Hansen. "The foundations of spectral computations via the solvability complexity index hierarchy." Journal of the European Mathematical Society (2022).
[9] Colbrook, Matthew, Andrew Horning, and Alex Townsend. "Computing spectral measures of self-adjoint operators." SIAM review 63.3 (2021): 489-524.
[10] Colbrook, Matthew J., Bogdan Roman, and Anders C. Hansen. "How to compute spectra with error control." Physical Review Letters 122.25 (2019): 250201.
[11] Colbrook, Mathew J. "On the computation of geometric features of spectra of linear operators on Hilbert spaces." Foundations of Computational Mathematics (2022): 1-82.
[12] Colbrook, Matthew J. "Computing spectral measures and spectral types." Communications in Mathematical Physics 384 (2021): 433-501.
[13] Colbrook, Matthew J., and Anders C. Hansen. "On the infinite-dimensional QR algorithm." Numerische Mathematik 143 (2019): 17-83.
[14] Colbrook, Matthew. "Pseudoergodic operators and periodic boundary conditions." Mathematics of Computation 89.322 (2020): 737-766.
[15] Colbrook, Matthew J., and Alex Townsend. "Avoiding discretization issues for nonlinear eigenvalue problems." arXiv preprint arXiv:2305.01691 (2023).
[16] Colbrook, Matthew, Andrew Horning, and Alex Townsend. "Resolvent-based techniques for computing the discrete and continuous spectrum of differential operators." XXI Householder Symposium on Numerical Linear Algebra. 2020.
[17] Johnstone, Dean, et al. "Bulk localized transport states in infinite and finite quasicrystals via magnetic aperiodicity." Physical Review B 106.4 (2022): 045149.
[18] Colbrook, Matthew J., et al. "Computing spectral properties of topological insulators without artificial truncation or supercell approximation." IMA Journal of Applied Mathematics 88.1 (2023): 1-42.
[19] Colbrook, Matthew J., and Andrew Horning. "Specsolve: spectral methods for spectral measures." arXiv preprint arXiv:2201.01314 (2022).
[20] Colbrook, Matthew J., and Alex Townsend. "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems." arXiv preprint arXiv:2111.14889 (2021).
[21] Colbrook, Matthew J., Lorna J. Ayton, and Máté Szöke. "Residual dynamic mode decomposition: robust and verified Koopmanism." Journal of Fluid Mechanics 955 (2023): A21.
[22] Colbrook, Matthew J. "The mpEDMD algorithm for data-driven computations of measure-preserving dynamical systems." SIAM Journal on Numerical Analysis 61.3 (2023): 1585-1608.
[23] Brunton, Steven L., and Matthew J. Colbrook. "Resilient Data-driven Dynamical Systems with Koopman: An Infinite-dimensional Numerical Analysis Perspective."
[24] Colbrook, Matthew J. "Computing semigroups with error control." SIAM Journal on Numerical Analysis 60.1 (2022): 396-422.
[25] Colbrook, Matthew J., and Lorna J. Ayton. "A contour method for time-fractional PDEs and an application to fractional viscoelastic beam equations." Journal of Computational Physics 454 (2022): 110995.


[^0]:    - C., "The foundations of infinite-dimensional spectral computations," PhD diss., University of Cambridge, 2020.

[^1]:    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.

    - Antun, C., Hansen, "Proving Existence Is Not Enough: : Mathematical Paradoxes Unravel the Limits of Neural Networks in Artificial Intelligence," SIAM News, May 2022.
    - Choi, "Some AI Systems May Be Impossible to Compute," IEEE Spectrum, March 2022.

