The difficulty of computing stable and accurate neural networks

On the barriers of deep learning & Smale's 18th problem

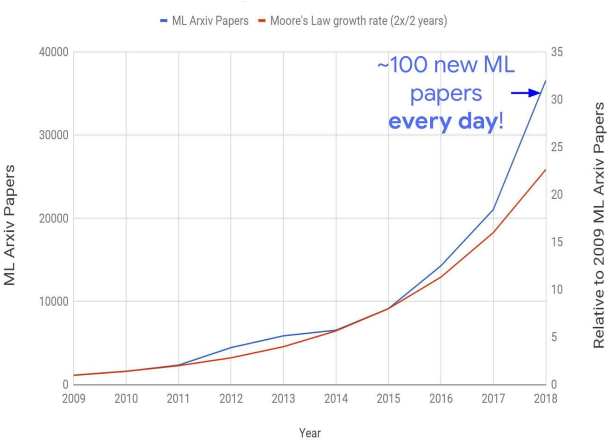
Matthew Colbrook
University of Cambridge

Smale's 18th problem*: *What are the limits of artificial intelligence?*

M. Colbrook, V. Antun, A. Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem*" (PNAS, 2022)

*Steve Smale's list of problems for the 21st century (requested by Vladimir Arnold), inspired by Hilbert's list.

Interest in deep learning exponentially growing



To keep up during first lockdown, would need to continually read a paper every 4 mins!

E.g., will AI replace standard algorithms in medical imaging?

nature > letters > article

a natureresearch journal

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Published: 22 March 2018

Image reconstruction by domain-transform manifold learning

Bo Zhu, Jeremiah Z. Liu, Stephen F. Cauley, Bruce R. Rosen & Matthew S. Rosen

Nature **555**, 487–492(2018) | Cite this article

Abstract

Image reconstruction is essential for imaging applications across the physical and life sciences, including optical and radar systems, magnetic resonance imaging, X-ray computed tomography, positron emission

Editorial Summary

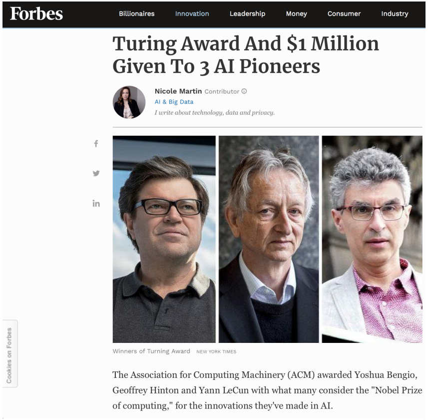
Machine learning improves image reconstruction

Reconstructing images from data, whether for medical or astronomical purposes, hinges on well-defined steps. The data sensor encodes an intermediate representation of the observed

show all

Claim: "superior immunity to noise and a reduction in reconstruction artefacts compared with conventional handcrafted reconstruction methods".

Very strong confidence in deep learning



Forbes Billionaires Innovation Leadership Money Consumer Industry

Turing Award And $1 Million Given To 3 AI Pioneers

Nicole Martin Contributor
AI & Big Data
I write about technology, data and privacy.

Winners of Turning Award NEW YORK TIMES

The Association for Computing Machinery (ACM) awarded Yoshua Bengio, Geoffrey Hinton and Yann LeCun with what many consider the "Nobel Prize of computing," for the innovations they've made in AI.

Cookies on Forbes

Geoffrey Hinton, The New Yorker, 04-17: "They should stop training radiologists now!"

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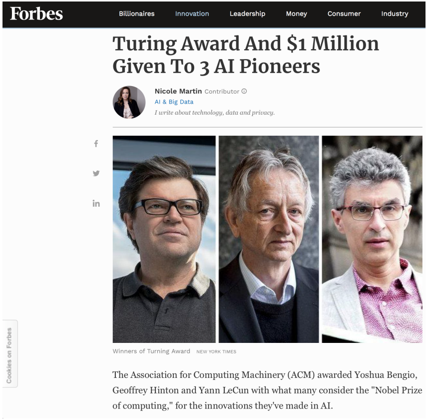
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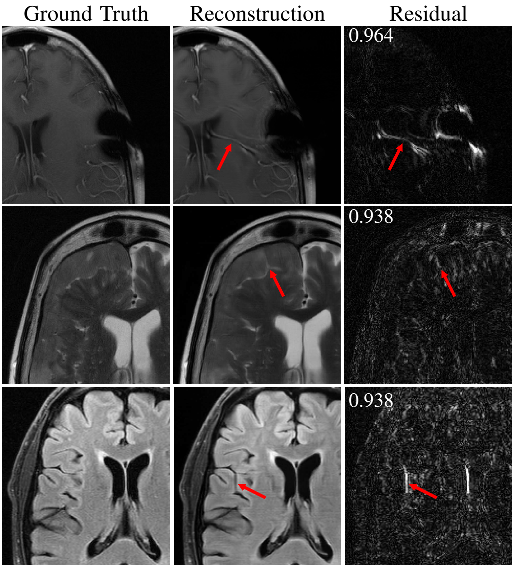
BUT . . .

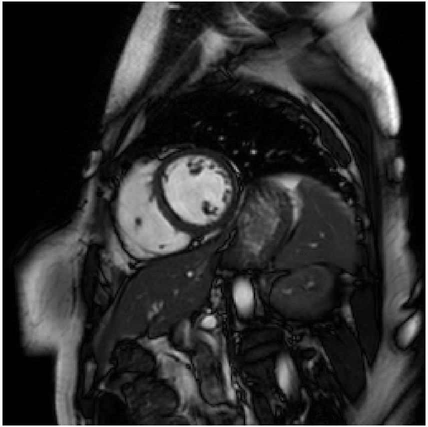
AI hallucinations (Facebook and NYU's 2020 FastMRI challenge)



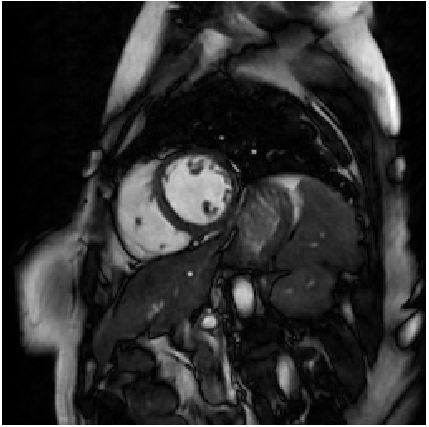
*"On AI, trust is a must, not a nice to have. High-risk AI systems will be subject to **strict obligations** before they can be put on the market: High level of **robustness**, **security** and **accuracy**."*
- Europ. Comm. outline for legal AI (April 2021).

Example of instabilities in inverse problems

$|x|$



$|\Psi(Ax)|$



Network (33% subsampling) from: J. Schlemper, J. Caballero, J. V. Hajnal, A. Price and D. Rueckert, '*A deep cascade of convolutional neural networks for MR image reconstruction*', in International conference on information processing in medical imaging, Springer, 2017, pp. 647–658.
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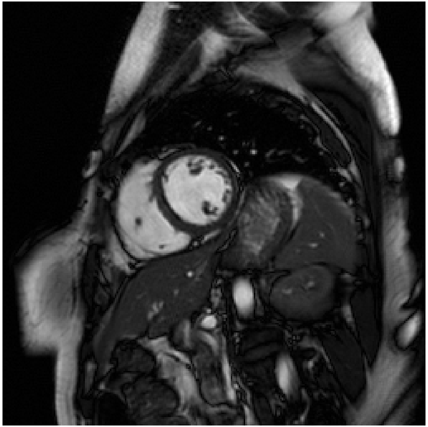
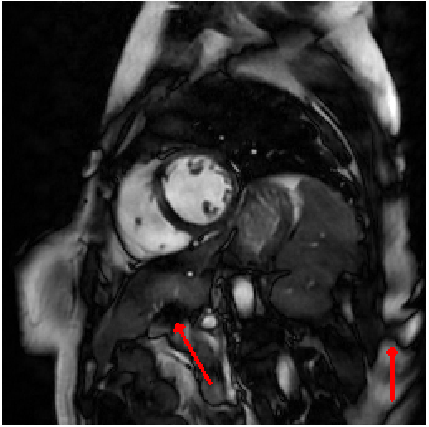
Example of instabilities in inverse problems

$|x + r_1|$



$|\Psi(A(x + r_1))|$



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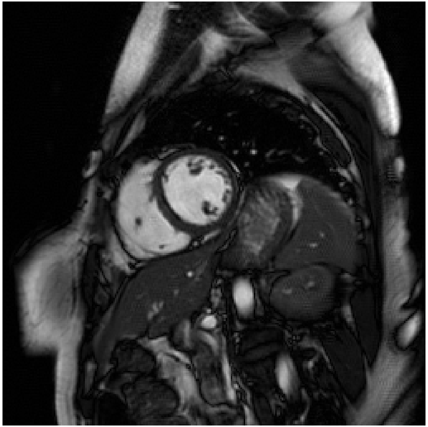
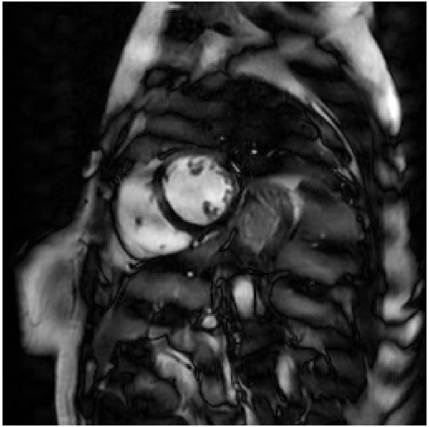
Example of instabilities in inverse problems

$|x + r_2|$



$|\Psi(A(x + r_2))|$



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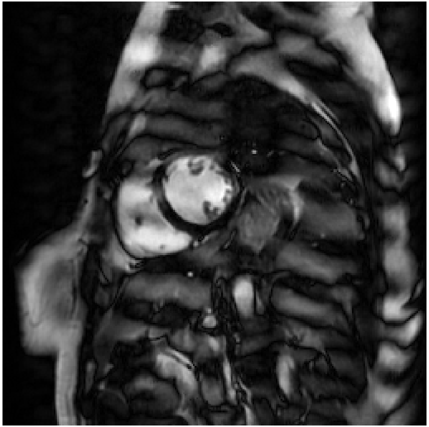
Example of instabilities in inverse problems

$|x + r_3|$

$|\Psi(A(x + r_3))|$



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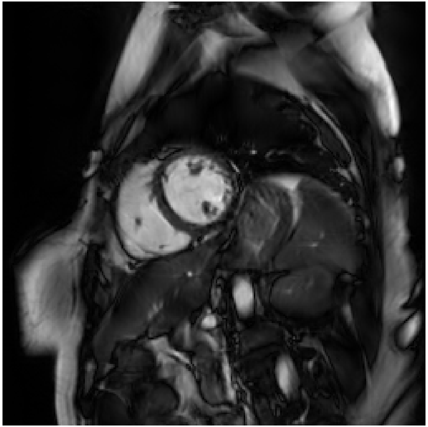
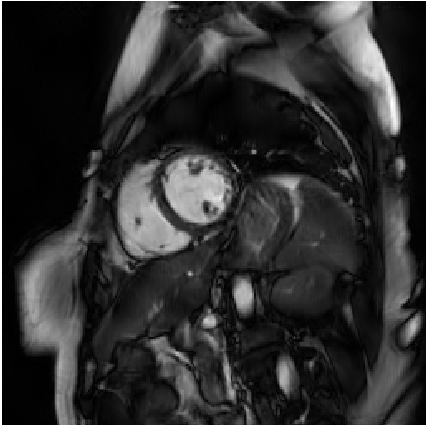
Reconstruction using state-of-the-art standard methods

SoA from Ax



SoA from $A(x + r_3)$



Smale's 18th prob.: What are the limits of artificial intelligence?

"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 (NYU, Facebook's chief AI scientist, Turing Award 2018)

"2021 was the year in which the wonders of artificial intelligence stopped being a story. Many of this year's top articles grappled with the **limits of deep learning** *(***today's dominant strand of AI***)."*

— IEEE Spectrum, 2021's Top Stories About AI (Dec. 2021)

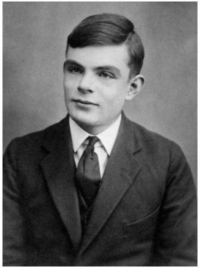
Echoes of an old story

Hilbert's vision (start of 20th century): secure foundations for all mathematics.

- Mathematics written in a precise language.
- Completeness: all true math. statements can be proven.
- Consistency: no contradiction can be obtained.
- Decidability: algorithm for deciding truth of math. statements.

Hilbert's 10th problem: *Provide an algorithm which, for any given polynomial equation with integer coefficients, can decide whether there is an integer-valued solution.*

Foundations ⇒ better understanding, feasible directions for techniques, new methods, . . .



Gödel (pioneer of **modern logic**) and Turing (pioneer of **modern computer science**):

- True statements in mathematics that cannot be proven!
- Computational problems that cannot be computed by an algorithm!

Hilbert's 10th problem: No such algorithm exists (1970, Matiyasevich).

A program for the foundations of DL and AI

A program determining the foundations/limitations of deep learning and AI is needed:

- Boundaries of methodologies.
- Universal/intrinsic boundaries (e.g., no algorithm can do it).

Key difference between existence and construction.

Two pillars of scientific computation:

- Stability
- Accuracy

GOAL of talk: Results in this direction for inverse problems.

Mathematical setup

Given $y = Ax + e$ recover $x \in \mathbb{C}^N$. $A \in \mathbb{C}^{m \times N}$, $m < N$ (e.g., MRI).

Outline:

- Paradox.
- Sufficient conditions and Fast Iterative REstarted NETworks (FIRENETs).
- Numerical examples (e.g., stability-accuracy trade-off).
- Approximate sharpness conditions and Weighted, Accelerated and Restarted Primal-dual (WARPd).

Can we train neural networks that solve (P_j)?

$$\min_{x\in\mathbb{C}^N} \|x\|_{\ell^1} \quad \text{subject to} \quad \|Ax-y\|_{\ell^2} \leq \eta \tag{P_1}$$

$$\min_{x\in\mathbb{C}^N} \lambda\|x\|_{\ell^1} + \|Ax-y\|_{\ell^2}^2 \tag{P_2}$$

$$\min_{x\in\mathbb{C}^N} \lambda\|x\|_{\ell^1} + \|Ax-y\|_{\ell^2} \tag{P_3}$$

Ξ = set of solutions.

Why P_j?

- Avoid bizarre, unnatural & pathological mappings: (P_j) well-understood & well-used!
- Simpler solution map than inverse problem $\Rightarrow$ stronger impossibility results.
- DL has also been used to speed up sparse regularization and tackle (P_j).

The set-up

$$A \in \mathbb{C}^{m\times N} \text{ (modality)}, \quad \mathcal{S} = \{y_k\}_{k=1}^R \subset \mathbb{C}^m \text{ (samples)}, \quad R < \infty$$

In practice, A not known exactly or cannot be stored to infinite precision.

Assume access to: $\{y_{k,n}\}_{k=1}^R$ and A_n (rational approximations, e.g., floats) such that

$$\|y_{k,n} - y_k\| \leq 2^{-n}, \quad \|A_n - A\| \leq 2^{-n}, \quad \forall n \in \mathbb{N}.$$

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

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

In a nutshell: allow access to arbitrary precision training data.

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In a nutshell: allow access to arbitrary precision training data.

Question: Given a collection Ω of $(A, \mathcal{S})$, does there exist a neural network approximating Ξ (solution map of (P_j)), and can it be trained by an algorithm?

What could go wrong?

$$\min_{x\in\mathbb{C}^N} \|x\|_{\ell^1} \quad \text{subject to} \quad \|Ax-y\|_{\ell^2} \leq \eta \qquad (P_1)$$

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(i) **Non-existence:** No neural network approximates Ξ.

(ii)

(iii)

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(ii) **Non-trainable:** $\exists$ a neural network that approximates Ξ, but it cannot be trained.

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(i) ~~**Non-existence:** No neural network approximates Ξ.~~

(ii) **Non-trainable:** $\exists$ a neural network that approximates Ξ, but it cannot be trained.

(iii) **Not practical:** $\exists$ a neural network that approximates Ξ, and an algorithm training it. However, the algorithm needs prohibitively many samples.

Paradox

Theorem

For (P_j), $N \geq 2$ *and* $m < N$. *Let* $K \geq 3$ *be a positive integer,* $L \in \mathbb{N}$. *Then there exists a* **well-conditioned** *class (condition numbers* ≤ 1*)* Ω *of elements* $(A, \mathcal{S})$ *s.t. (*Ω **fixed** *in what follows):*

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(i) *There* **does not exist any algorithm** *that, given a training set* $\iota_{A,\mathcal{S}}$, *produces a neural network* $\phi_{A,\mathcal{S}}$ *with*

$$\min_{y \in \mathcal{S}} \inf_{x^* \in \Xi(A,y)} \|\phi_{A,\mathcal{S}}(y) - x^*\|_{\ell^2} \leq 10^{-K}, \quad \forall (A, \mathcal{S}) \in \Omega. \tag{1}$$

Furthermore, for any $p > 1/2$, **no probabilistic algorithm** *can produce a neural network* $\phi_{A,\mathcal{S}}$ *such that (1) holds with probability at least* p.

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(ii) *There* **exists an algorithm** *that produces a neural network* $\phi_{A,\mathcal{S}}$ *such that*

$$\max_{y \in \mathcal{S}} \inf_{x^* \in \Xi(A,y)} \|\phi_{A,\mathcal{S}}(y) - x^*\|_{\ell^2} \leq 10^{-(K-1)}, \quad \forall (A, \mathcal{S}) \in \Omega.$$

However, for any such algorithm (even probabilistic), $M \in \mathbb{N}$ *and* $p \in \left[0, 1 - \frac{1}{N+1-m}\right)$, *there exists a training set* $\iota_{A,\mathcal{S}}$ *such that for all* $y \in \mathcal{S}$,

$$\mathbb{P}\left(\inf_{x^* \in \Xi(A,y)} \|\phi_{A,\mathcal{S}}(y) - x^*\|_{\ell^2} > 10^{-(K-1)} \text{ or size of training data needed} > M \right) > p.$$

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(iii) *There* **exists an algorithm** *using only* L *training data from each* $\iota_{A,\mathcal{S}}$ *that produces a neural network* $\phi_{A,\mathcal{S}}(y)$ *such that*

$$\max_{y \in \mathcal{S}} \inf_{x^* \in \Xi(A,y)} \|\phi_{A,\mathcal{S}}(y) - x^*\|_{\ell^2} \leq 10^{-(K-2)}, \quad \forall (A, \mathcal{S}) \in \Omega.$$

In words . . .

Nice classes Ω where stable and accurate neural networks exist. But:

- K digits: $\nexists$ training algorithm for neural network.
- $K-1$ digits: $\exists$ training algorithm for neural network,
  but any such algorithm needs arbitrarily many training data.
- $K-2$ digits: $\exists$ training algorithm for neural network using L training samples.

Independent of neural network architecture - universal barrier.

Existence vs computation (universal approximation theorems **not** enough).

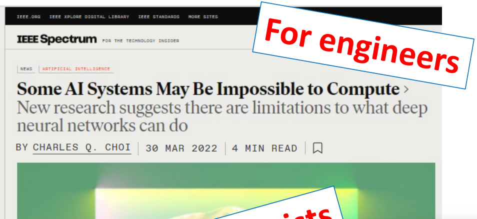
Conclusion: Theorems on existence of neural networks may have little to do with the neural networks produced in practice . . .

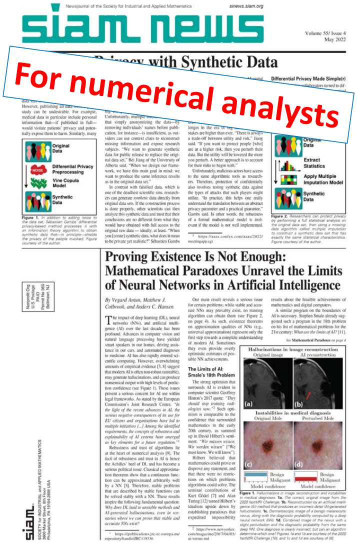
Numerical example: fails with training methods

$\text{dist}(\Psi_{A_n}(y_n), \Xi(A, y))$	$\text{dist}(\Phi_{A_n}(y_n), \Xi(A, y))$	$\|A_n - A\| \leq 2^{-n}$ $\|y_n - y\|_{\ell^2} \leq 2^{-n}$	10^{-K}
0.2999690	0.2597827	$n = 10$	10^{-1}
0.3000000	0.2598050	$n = 20$	10^{-1}
0.3000000	0.2598052	$n = 30$	10^{-1}
0.0030000	0.0025980	$n = 10$	10^{-3}
0.0030000	0.0025980	$n = 20$	10^{-3}
0.0030000	0.0025980	$n = 30$	10^{-3}
0.0000030	0.0000015	$n = 10$	10^{-6}
0.0000030	0.0000015	$n = 20$	10^{-6}
0.0000030	0.0000015	$n = 30$	10^{-6}

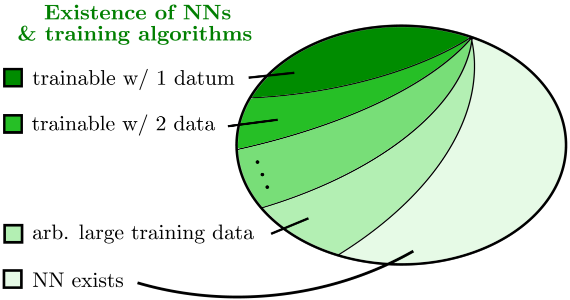
Table: (**Impossibility of computing the existing neural network to arbitrary accuracy**). Matrix $A \in \mathbb{C}^{19\times 20}$ constructed from discrete cosine transform, $R = 8000$, solutions are 6-sparse. LISTA (learned iterative shrinkage thresholding algorithm) Ψ_{A_n}, and FIRENETs Φ_{A_n}. The table shows the shortest ℓ^2 distance between the output from the networks and the true minimizer of the problem $\min_{x\in\mathbb{C}^N} \|x\|_{\ell^1} + \|Ax - y\|_{\ell^2}$, for different values of n and K.

A paradox relevant to applications





The world of neural networks



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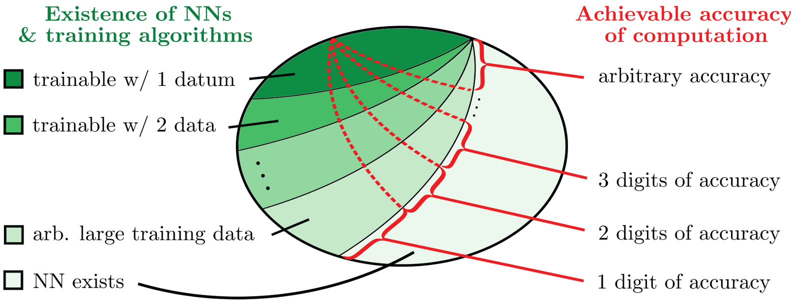


Need: Classification theory saying what can/cannot be done.

Example:

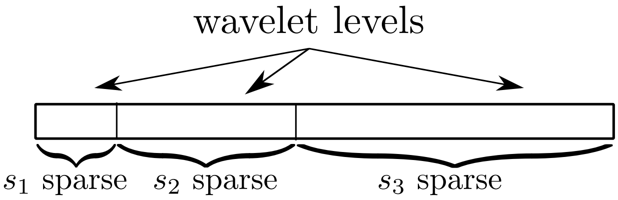
$$\hat{x} \in \operatorname{argmin} f(x), \quad f^* = \min f(x)$$

Problem: $f(x) \leq f^* + \epsilon$ does not in general imply x is close to set of minimizers.

Question: Can we find 'good' input classes where

$$f(x) \leq f^* + \epsilon \implies \inf_{\hat{x} \in \operatorname{argmin} f(x)} \|x - \hat{x}\| \lesssim \epsilon?$$

State-of-the-art model for sparse regularisation



$\mathbf{M} = (M_1, \ldots, M_r) \in \mathbb{N}^r$ and $\mathbf{s} = (s_1, \ldots, s_r) \in \mathbb{Z}^r_{\geq 0}$. $x \in \mathbb{C}^N$ is $(\mathbf{s}, \mathbf{M})$-sparse in levels if

$$|\mathrm{supp}(x) \cap \{M_{k-1} + 1, \ldots, M_k\}| \leq s_k, \quad k = 1, \ldots, r.$$

Denote set of $(\mathbf{s}, \mathbf{M})$-sparse vectors by $\Sigma_{\mathbf{s},\mathbf{M}}$, define

$$\sigma_{\mathbf{s},\mathbf{M}}(x)_{\ell^1} = \inf\{\|x - z\|_{\ell^1} : z \in \Sigma_{\mathbf{s},\mathbf{M}}\}.$$

The robust nullspace property

Definition: $A \in \mathbb{C}^{m\times N}$ satisfies the **robust null space property in levels (rNSPL)** of order $(\mathbf{s}, \mathbf{M})$ with constants $\rho \in (0,1)$ and $\gamma > 0$ if for any $(\mathbf{s}, \mathbf{M})$ support set Δ,

$$\|x_\Delta\|_{\ell^2} \leq \frac{\rho \|x_{\Delta^c}\|_{\ell^1}}{\sqrt{r(s_1 + \ldots + s_r)}} + \gamma \|Ax\|_{\ell^2}, \qquad \forall x \in \mathbb{C}^N.$$

Objective function: $f(x) = \lambda \|x\|_{\ell^1} + \|Ax - y\|_{\ell^2}$

$$\text{rNSPL} \Rightarrow \|z - x\|_{\ell^2} \lesssim \underbrace{\sigma_{\mathbf{s},\mathbf{M}}(x)_{\ell^1} + \|Ax - y\|_{\ell^2}}_{\text{“small”}} + \underbrace{\left(\lambda\|z\|_{\ell^1} + \|Az - y\|_{\ell^2} - \lambda\|x\|_{\ell^1} - \|Ax - y\|_{\ell^2}\right)}_{f(z)-f(x) \text{ objective function difference}},$$

In a nutshell: control $\|z - x\|_{\ell^2}$ by $f(z) - f(x)$, up to small approximation term.

Fast Iterative REstarted NETworks (FIRENETs)

Simplified version of Theorem: *We provide an algorithm such that:*

Input: *Sparsity parameters* $(\mathbf{s}, \mathbf{M})$, $A \in \mathbb{C}^{m \times N}$ *satisfying the rNSPL with constants* $0 < \rho < 1$ *and* $\gamma > 0$, $n \in \mathbb{N}$ *and positive* $\{\delta, b_1, b_2\}$.

Output: *A neural network* ϕ_n *with* $\mathcal{O}(n)$ *layers and width* $2(N+m)$ *such that:*

For any $x \in \mathbb{C}^N$ *and* $y \in \mathbb{C}^m$ *with*

$$\underbrace{\sigma_{\mathbf{s},\mathbf{M}}(x)_{\ell^1}}_{\text{distance to sparse in levels vectors}} + \underbrace{\|Ax - y\|_{\ell^2}}_{\text{noise of measurements}} \lesssim \delta, \quad \|x\|_{\ell^2} \lesssim b_1, \quad \|y\|_{\ell^2} \lesssim b_2,$$

we have the following **stable** *and* **exponential convergence** *guarantee in* n

$$\|\phi_n(y) - x\|_{\ell^2} \lesssim \delta + e^{-n}.$$

Demonstration of convergence

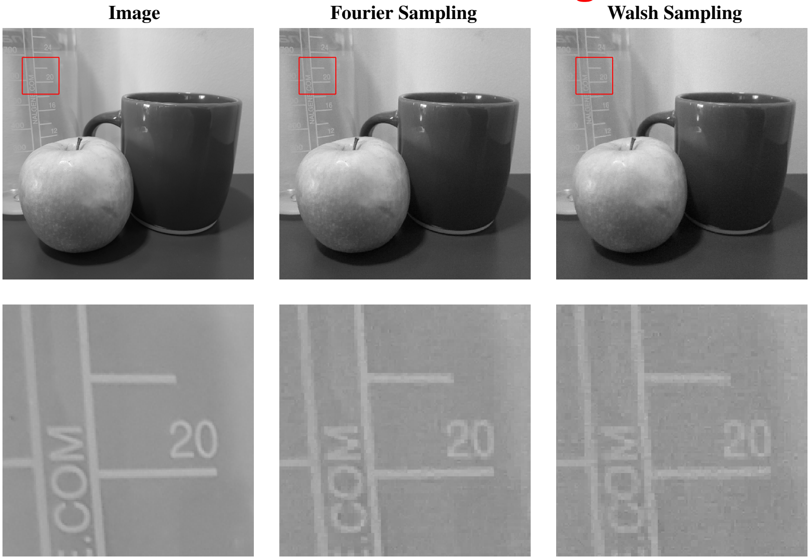
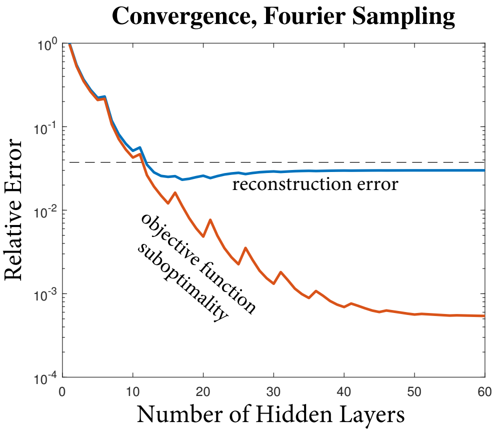
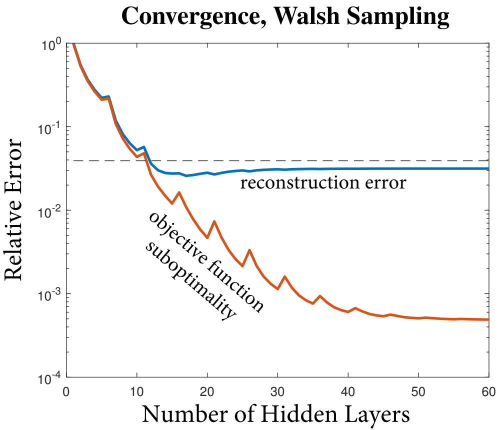


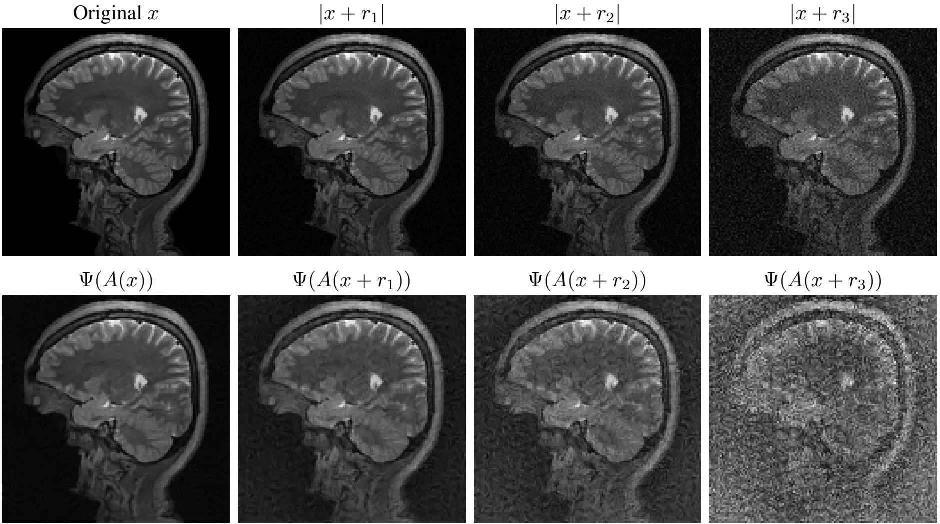
Figure: Images corrupted with 2% Gaussian noise and reconstructed using 15% sampling.

Demonstration of convergence



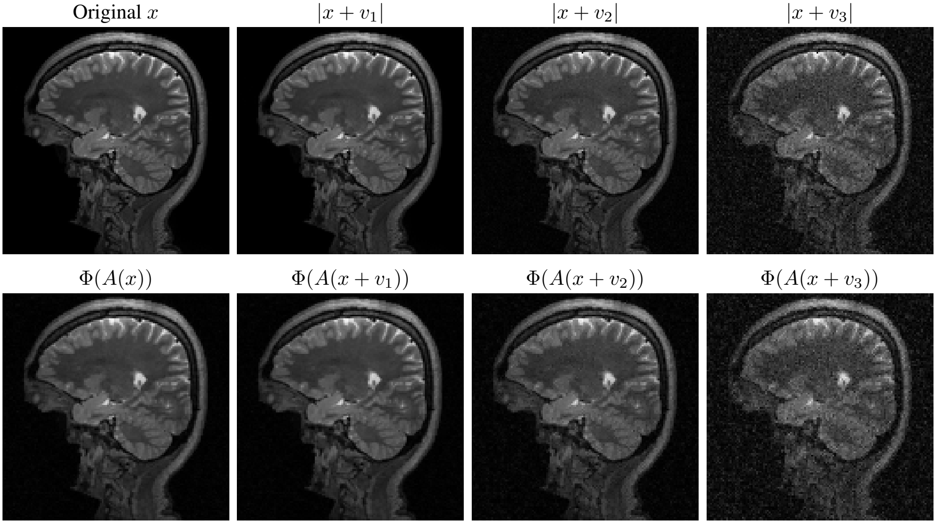


Stable? AUTOMAP ✗



· V. Antun et al. "*On instabilities of deep learning in image reconstruction and the potential costs of AI*," PNAS, 2021.
· B. Zhu et al. "*Image reconstruction by domain-transform manifold learning*," Nature, 2018.

Stable? FIRENETs ✓



· M. Colbrook, V. Antun, A. Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem*," PNAS, 2022.

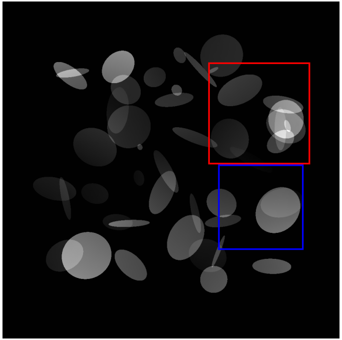
Adding FIRENET layers stabilizes AUTOMAP

$|x + \mathrm{e}_3|$ $\Psi(\tilde{y}), \tilde{y} = A(x + \mathrm{e}_3)$ $\Phi(\tilde{y}, \Psi(\tilde{y}))$

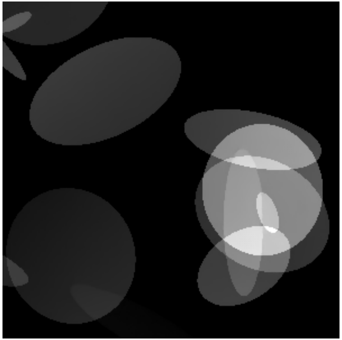
· M. Colbrook, V. Antun, A. Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem*," PNAS, 2022.

Stability vs. accuracy tradeoff

Original x
(full size)



Original
(cropped, red frame)

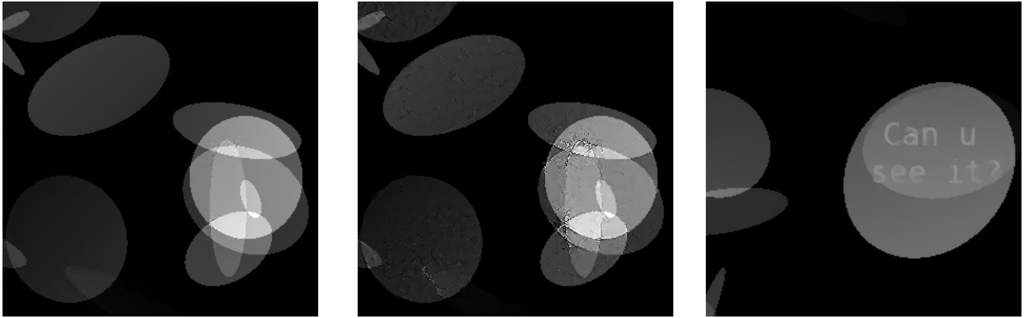


Original + detail ($x + h_1$)
(cropped, blue frame)

· M. Colbrook, V. Antun, A. Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem*," PNAS, 2022.

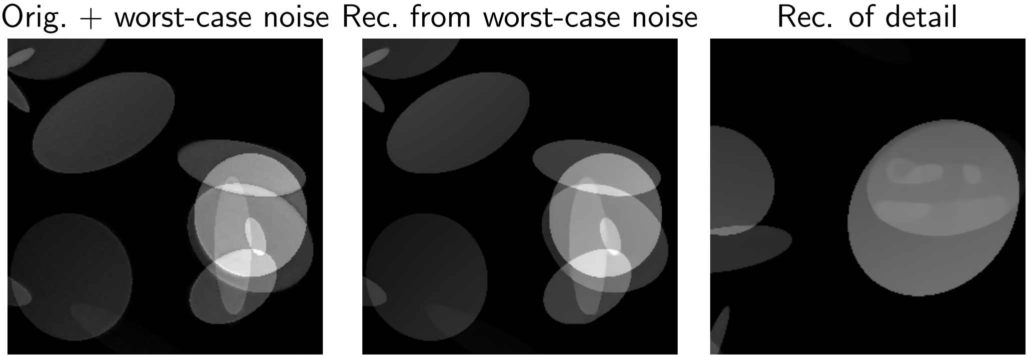
U-net trained without noise

Orig. + worst-case noise Rec. from worst-case noise Rec. of detail



· M. Colbrook, V. Antun, A. Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem*," PNAS, 2022.

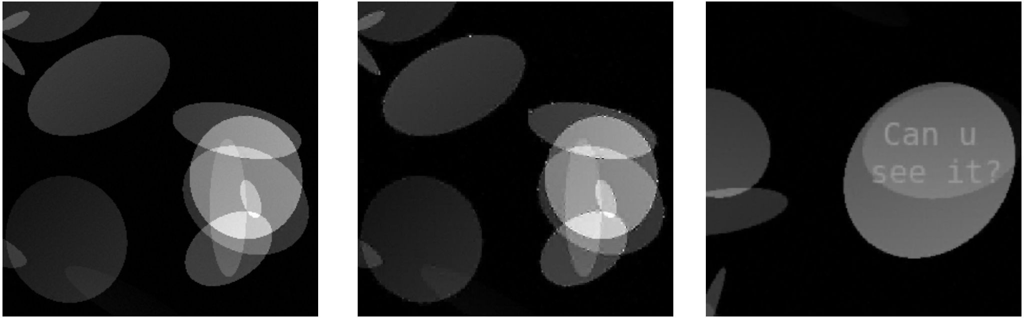
U-net trained with noise



· M. Colbrook, V. Antun, A. Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem*," PNAS, 2022.

FIRENET

Orig. + worst-case noise | Rec. from worst-case noise | Rec. of detail



· M. Colbrook, V. Antun, A. Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem*," PNAS, 2022.

Broader framework: approximate sharpness conditions

Problem: Given $y = Ax + e \in \mathbb{C}^m$, recover $x \in \mathbb{C}^N$.

Optimization: $\min_{x\in\mathbb{C}^N} \mathcal{J}(x) + \|Bx\|_{\ell^1}$ s.t. $\|Ax - y\|_{\ell^2} \leq \epsilon$, $B \in \mathbb{C}^{q\times N}$.

Assume: $\|\hat{x} - x\|_{\ell^2} \leq C_1\Big[\underbrace{\mathcal{J}(\hat{x}) + \|B\hat{x}\|_{\ell^1} - \mathcal{J}(x) - \|Bx\|_{\ell^1}}_{\text{objective function difference}} + C_2\underbrace{\left(\|A\hat{x} - y\|_{\ell^2} - \epsilon\right)}_{\text{feasibility gap}} + \underbrace{c(x,y)}_{\text{approx. term}}\Big]$.

Examples: Sparse vector recovery, low-rank matrix recovery, matrix completion, ℓ^1-analysis problems, TV minimization, mixed regularization problems, ...

Simplified version of Theorem: *Let $\delta > 0$. We provide a neural network ϕ of depth $\mathcal{O}(\log(\delta^{-1}))$ and width $\mathcal{O}(N + m + q)$ such that for all $(x, y) \in \mathbb{C}^N \times \mathbb{C}^m$*

$$\|Ax - y\|_{\ell^2} \leq \epsilon \text{ and } c(x,y) \leq \delta \quad \Rightarrow \quad \|\phi(y) - x\|_{\ell^2} \lesssim \delta.$$

· M. Colbrook "*WARPd: A linearly convergent first-order method for inverse problems with approximate sharpness conditions.*"

Concluding remarks

Need for foundations in AI/deep learning.

- **Paradox:** 'Nice' inverse problems where stable & accurate neural network exists but cannot be trained! $\forall K \in \mathbb{Z}_{\geq 3}$, $\exists$ classes s.t.:
  - (i) Algorithms may compute neural networks to $K-1$ digits of accuracy, but not K.
  - (ii) Achieving $K-1$ digits of accuracy requires arbitrarily many training data.
  - (iii) Achieving $K-2$ correct digits requires only one training datum.
- Specific conditions $\Rightarrow$ **FIRENETs** exp. convergence + withstand adversarial attacks. **WARPd** provides accelerated recovery under an *approximate sharpness condition*. WARPd $\underset{\text{unrolled}}{\Rightarrow}$ FIRENETs.
- **Trade-off** between stability and accuracy in deep learning.

Open question: How do we *optimally* traverse the *stability* & *accuracy* trade-off? Existence is not enough!