Can stable and accurate neural networks always be computed?

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Joint work with: Vegard Antun (Oslo), Anders Hansen (Cambridge)

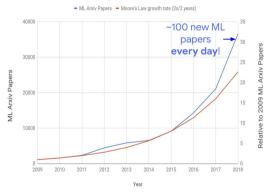
Based on: M. Colbrook, V. Antun, A. Hansen, "Can stable and accurate neural networks be computed? - On the barriers of deep learning and Smale's 18th problem"

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

Code: www.github.com/Comp-Foundations-and-Barriers-of-AI/firenet

Interest in deep learning unprecedented and exponentially growing

Machine Learning Arxiv Papers per Year



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

The ubiquity of AI

Al techniques are replacing humans in problem solving:

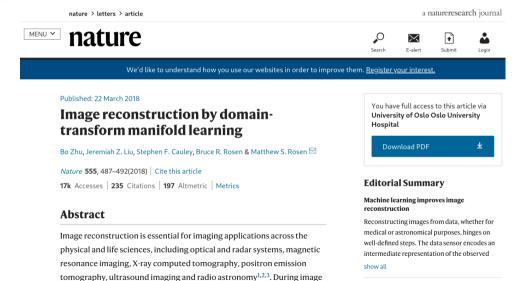
- Self-driving vehicles
- ▶ Automated diagnosis in medicine and automated decision processes
- Automated weapon systems
- Music composition
- Call centres
- ► Any security system based on face or voice recognition
- Mathematical proofs

Al techniques are replacing established algorithms in science:

- ► Medical imaging (MRI, CT, etc)
- Microscopy
- ► Imaging problems in general
- Radar, sonar, etc.
- Methods for solving PDEs

Will AI replace standard algorithms in medical imaging?

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



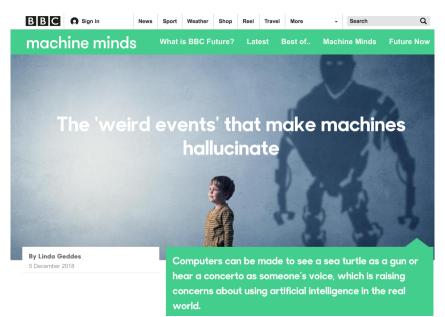
Very strong confidence in deep learning

The New Yorker quotes Geoffrey Hinton (April 2017):

"They should stop training radiologists now."

BUT...

DANGER: Al generated hallucinations



The danger of false negatives

Uber's self-driving car saw the pedestrian but didn't swerve - report

Tuning of car's software to avoid false positives blamed, as US National Transportation Safety Board investigation continues



▲ Uber's modified Volvo XC90 SUV detected but did not react to the crossing pedestrian in first self-driving car fatality, report says, Photograph; Volvo

An Uber self-driving test car which killed a woman crossing the street detected her but decided not to react immediately, a report has said.

The car was travelling at 40mph (64km/h) in self-driving mode when it collided with 49-year-old Elaine Herzberg at about 10pm on 18 March. Herzberg was pushing a bicycle across the road outside of a crossing. She later died from her injuries.

Although the car's sensors detected Herzberg, its software which decides how it should react was tuned too far in favour of ignoring objects in its path which might be "false positives" (such as plastic bags), according to a report from the Information. This meant the modified Volvo XC90 did not react fast enough.

Deep Fool

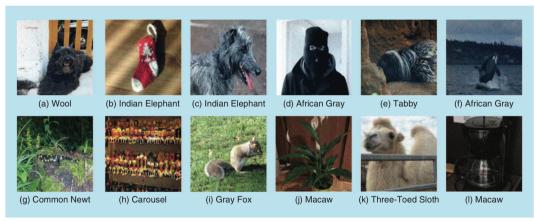
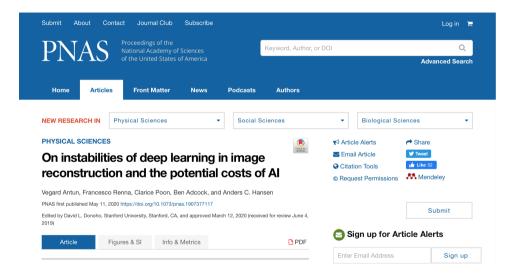
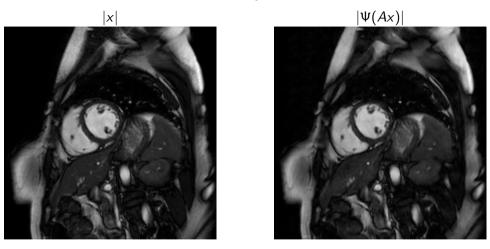
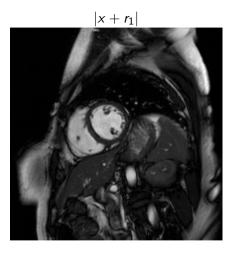


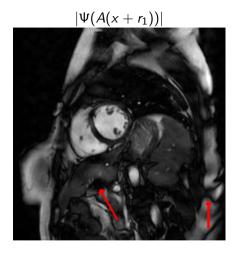
FIGURE 4. Examples of natural images perturbed with the universal perturbation and their corresponding estimated labels with GoogLeNet. (a)—(h) Images belonging to the ILSVRC 2012 validation set. (i)—(l) Personal images captured by a mobile phone camera. (Figure used courtesy of [22].)

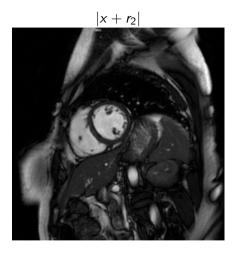
DL is also unstable in inverse problems!

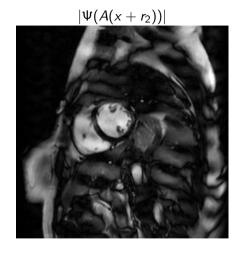


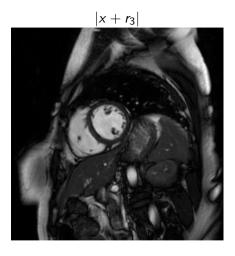


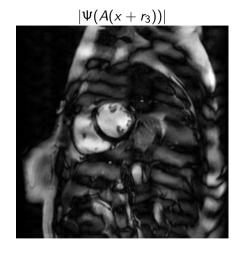




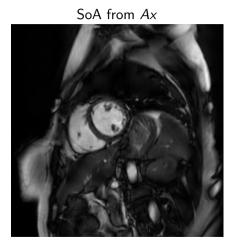


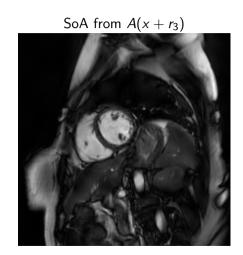




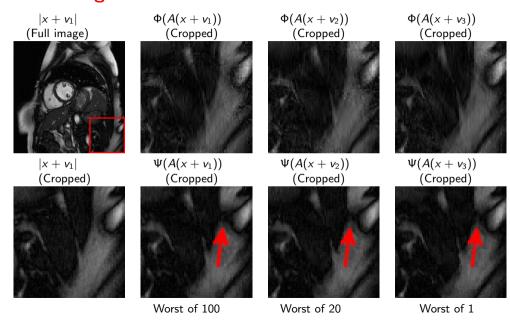


Reconstruction using state-of-the-art standard methods





Al generated hallucinations with random noise



Facebook and NYU's 2020 FastMRI challenge

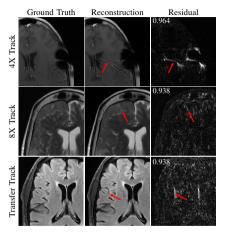


Fig. 6. Examples of reconstruction hallucinations among challenge submissions with SSIM scores over residual plots (residuals magnified by 5). (top) A 4X submission from Neurospin generated a false vessel, possibly related to susceptibilities introduced by surgical staples, (middle) An 8X submission from ATB introduced a linear bright signal mimicking a cleft of cerebrospinal fluid, as well as blurring of the boundaries of the extra-axial mass. (bottom) A submission from ResoNNance introduced a false sulcus or prominent vessel.

Optimism: Echoes of an old story

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

- ► Mathematics should be written in a precise language, manipulated according to well defined rules.
- Completeness: a proof that all true mathematical statements can be proved in the formalism.
- Consistency: a proof that no contradiction can be obtained in the formalism of mathematics.
- Decidability: an algorithm for deciding the truth or falsity of any mathematical statement.



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

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





Gödel (father of **modern logic**) and Turing (father of **modern computer science**) turned Hilbert's optimism upside down:

- ► There exist true statements in mathematics that cannot be proven.
- ► There exists 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 Al

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

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).

There is a key difference between existence and construction here.

Need to also incorporate two pillars of numerical analysis:

- Stability
- Accuracy

GOAL for rest of talk: Develop some results in this direction for inverse problems.

*Steve Smale composed a list of problems for the 21st century in reply to a request of Vladimir Arnold inspired by Hilbert's list.

Mathematical setup

Given measurements y = Ax + e recover $x \in \mathbb{C}^N$.

- $\triangleright x \in \mathbb{C}^N$ be an unknown vector,
- $ightharpoonup A \in \mathbb{C}^{m \times N}$ be a matrix (m < N) describing modality (e.g. MRI), and
- ightharpoonup y = Ax + e the noisy measurements of x.

Outline:

- Fundamental barriers
- ► Sufficient conditions and Fast Iterative REstarted NETworks (FIRENETs)
- Balancing stability and accuracy

Can we compute neural networks that solve (P_j) ?

Sparse regularisation (benchmark problem):

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

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

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

Denote the **minimising** vectors by Ξ .

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

The set-up

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

In practice, the matrix A is 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

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

 $\text{And } \{x_{k,n}\}_{k=1}^R \text{ such that } \inf_{x^* \in \Xi(A_n,y_{k,n})} \|x_{k,n} - x^*\| \leq 2^{-n}, \quad \forall n \in \mathbb{N}.$

Training set associated with $(A, S) \in \Omega$ is

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

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, S), does there <u>exist</u> a neural network approximating Ξ (solution map of (P_j)), and <u>can it be trained</u> by an algorithm?

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

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(i) There does not exist a neural network that approximates the function we are interested in.

(ii)

(iii)

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- (ii) There does exist a neural network that approximates the function, however, there does not exist an algorithm that can construct the neural network.

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- (i) There does not exist a neural network that approximates the function we are interested in.
- (ii) There does exist a neural network that approximates the function, however, there does not exist an algorithm that can construct the neural network.
- (iii) There does exist a neural network that approximates the function, and an algorithm to construct it. However, the algorithm will need prohibitively many samples.

Bad news - can't necessarily approximate such a neural network

Theorem

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

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

$$\min_{\substack{y \in \mathcal{S} \ x^* \in \Xi(A,y)}} \|\phi_{A,\mathcal{S}}(y) - x^*\|_{l^2} \le 10^{-K}, \quad \forall (A,\mathcal{S}) \in \Omega. \tag{1}$$
for any $n > 1/2$, no probabilistic algorithm can produce a neural network $\phi_{A,\mathcal{S}}$.

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

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

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

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

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

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

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

In words...

Nice classes Ω where one can prove NNs with great approximation qualities exist. But:

- ▶ No algorithm, even randomised can train (or compute) such a NN accurate to *K* digits with probability greater than 1/2.
- There exists a deterministic algorithm that computes a NN with K-1 correct digits, but any such (even randomised) algorithm needs arbitrarily many training data.
- ▶ There exists a deterministic algorithm that computes a NN with K-2 correct digits using no more than L training samples.

Result independent of neural network architecture - a universal barrier.

Existence vs computation (universal approximation/interpolation 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

$dist(\Psi_{A_n}(y_n),\Xi_3(A,y))$	$\operatorname{dist}(\Phi_{A_n}(y_n),\Xi_3(A,y))$	$ A_n - A \le 2^{-n}$ $ y_n - y _{l^2} \le 2^{-n}$	10 ^{-K}	Ω_K
0.2999690	0.2597827	n = 10	10^{-1}	K = 1
0.3000000	0.2598050	n = 20	10^{-1}	K = 1
0.3000000	0.2598052	n = 30	10^{-1}	K = 1
0.0030000	0.0025980	n = 10	10^{-3}	K=3
0.0030000	0.0025980	n = 20	10^{-3}	K=3
0.0030000	0.0025980	n = 30	10^{-3}	K=3
0.000030	0.000015	n = 10	10^{-6}	K = 6
0.0000030	0.0000015	n = 20	10^{-6}	K = 6
0.0000030	0.0000015	n = 30	10^{-6}	K = 6

Table: (Impossibility of computing the existing neural network to arbitary accuracy). A constructed from discrete cosine transform, R=8000, N=20, m=19, solutions are 6-sparse. We demonstrate the impossibility statement (i) on FIRENETs Φ_{A_n} , and LISTA (learned iterative shrinkage thresholding algorithm) networks Ψ_{A_n} . The table shows the shortest I^2 distance between the output from the networks, and the true minimizer of the problem (P_3) , with $w_I=1$ and $\lambda=1$, for different values of n and K.

Can we avoid this?

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

Question: Can we find 'good' input classes where

$$f(x) < f^* + \epsilon \implies ||x - \hat{x}|| \lesssim \epsilon$$

We shall see that the answer is yes!

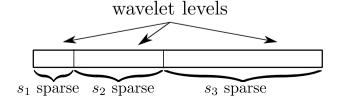
State-of-the-art model for sparse regularisation

Definition [Sparsity in levels]: Let $\mathbf{M} = (M_1, \dots, M_r) \in \mathbb{N}^r$, where $1 \leq M_1 < \dots < M_r = N$, and $\mathbf{s} = (s_1, \dots, s_r) \in \mathbb{N}_0^r$, where $s_k \leq M_k - M_{k-1}$ for $k = 1, \dots, r$ and $M_0 = 0$. A vector $x \in \mathbb{C}^N$ is (\mathbf{s}, \mathbf{M}) -sparse in levels if

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

The total sparsity is $s = s_1 + ... + s_r$. We denote the set of (s, M)-sparse vectors by $\Sigma_{s,M}$. We also define the following measure of distance of a vector x to $\Sigma_{s,M}$ by

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



The robust nullspace property

Definition [weighted rNSP in levels]: Let (\mathbf{s}, \mathbf{M}) be local sparsities and sparsity levels respectively. For weights $\{w_i\}_{i=1}^N$ $(w_i>0)$, we say that $A\in\mathbb{C}^{m\times N}$ satisfies the weighted robust null space property in levels (weighted rNSPL) of order (\mathbf{s}, \mathbf{M}) with constants $0<\rho<1$ and $\gamma>0$ if for any (\mathbf{s}, \mathbf{M}) support set Δ ,

$$\|x_{\Delta}\|_{l^2} \leq \frac{\rho \|x_{\Delta^c}\|_{l^1_w}}{\sqrt{\xi}} + \gamma \|Ax\|_{l^2}, \quad \text{for all } x \in \mathbb{C}^N.$$

$$\begin{split} \xi \coloneqq \sum_{k=1}^{r} w_{(k)}^{2} s_{k}, \quad \zeta \coloneqq \min_{k=1,\ldots,r} w_{(k)}^{2} s_{k}, \quad \kappa \coloneqq \frac{\xi}{\zeta}. \\ \text{rNSPL} \Rightarrow \|z_{1} - z_{2}\|_{l^{2}} \lesssim \underbrace{\sigma_{\textbf{s},\textbf{M}}(z_{2})_{l_{w}^{1}} + \|Az_{2} - y\|_{l^{2}}}_{\text{"small"}} \\ + \underbrace{\left(\lambda \|z_{1}\|_{l_{w}^{1}} + \|Az_{1} - y\|_{l^{2}} - \lambda \|z_{2}\|_{l_{w}^{1}} - \|Az_{2} - y\|_{l^{2}}\right)}_{f(z_{1}) - f(z_{2}) \text{ objective function difference}}, \end{split}$$

Main result

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

Input: Sparsity parameters (**s**, **M**), weights $\{w_i\}_{i=1}^N$, $A \in \mathbb{C}^{m \times N}$ (with the input A given by $\{A_i\}$) 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 the following property.

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

$$|\sigma_{\mathbf{s},\mathbf{M}}(x)|_{I_{\mathbf{w}_{j}}^{1}} + ||Ax - y||_{I_{j}^{2}} \lesssim \delta, ||x||_{I_{j}^{2}} \lesssim b_{1}, ||y||_{I_{j}^{2}} \lesssim b_{2},$$

distance to sparse in levels vectors noise of measurements

we have the following stable and exponential convergence guarantee in n

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

More detailed comments

- Architecture inspired by restarted & reweighted unrolling of primal-dual algorithm.
- ▶ As well as stability, rNSPL allows exponential convergence.
- Naive unrolling gives slow convergence $\mathcal{O}(\delta + n^{-1})$.
- ▶ If we do not know constants for rNSPL, can perform log-scale grid search for suitable parameters (increase width of layers by a factor of log(n)).
- ightharpoonup Error bounded when approximately applying layers of NNs \Rightarrow numerical stability.

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

Example in image recovery

Theorem

Consider recovering wavelet coeffs. $x = \Psi c$ of $c \in \mathbb{C}^{K^d}$ from subsampled noisy Fourier or Walsh measurements $y = DP_{\mathcal{I}}Vc + e$. Let $A = DP_{\mathcal{I}}V\Psi^*$, $m = |\mathcal{I}|$, $\epsilon_{\mathbb{P}} \in (0,1)$.

(i) If $\mathcal I$ is a random sampling pattern drawn according to strategy in paper, and

$$m \gtrsim (s_1 + \cdots + s_r) \cdot \mathcal{L}.$$

Then with prob. $1 - \epsilon_{\mathbb{P}}$, A satisfies wrNSPL of order (\mathbf{s}, \mathbf{M}) , $(\rho, \gamma) = (1/2, \sqrt{2})$.

(ii) For any $\delta \in (0,1)$, let $\mathcal{J}(\delta,\mathbf{s},\mathbf{M},w)$ be the set of all $y = Ax + e \in \mathbb{C}^m$ where

$$||x||_{l^2} \le 1$$
, $\max \left\{ \sigma_{s,M}(x)_{l_w^1}, ||e||_{l^2} \right\} \le \delta.$ (2)

We provide an algorithm that constructs a NN ϕ with $\mathcal{O}(\log(\delta^{-1}))$ hidden layers (width bounded by 2(N+m)) s.t. with probability at least $1-\epsilon_{\mathbb{P}}$,

$$\|\phi(y)-c\|_{l^2}\lesssim \delta, \quad \forall y=Ax+e\in \mathcal{J}(\delta,\mathbf{s},\mathbf{M},w).$$

Demonstration of convergence Age Fourier Sampling Walsh Sa

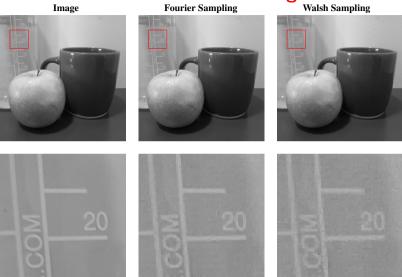
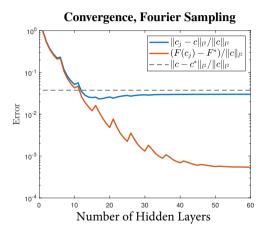
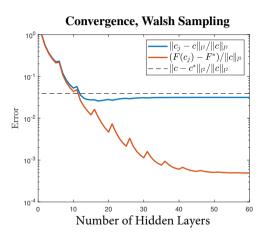


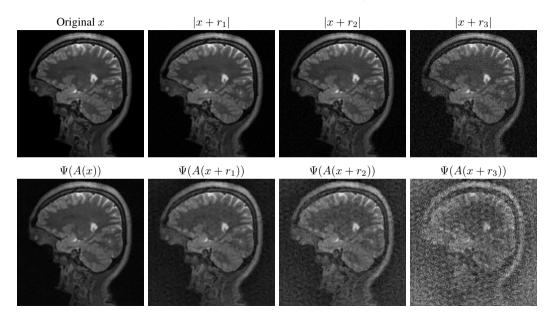
Figure: Images corrupted with 2% Gaussian noise and reconstructed using 15% sampling.

Demonstration of convergence

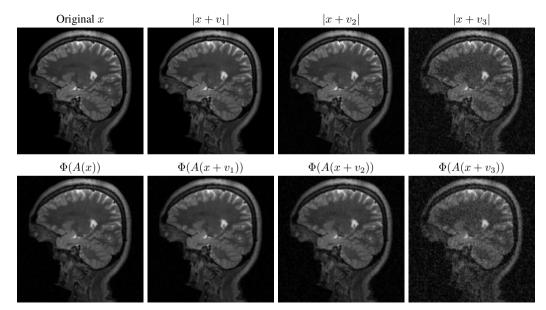




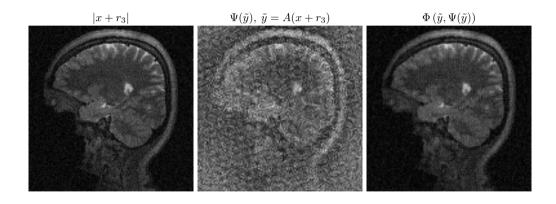
Stable? AUTOMAP X



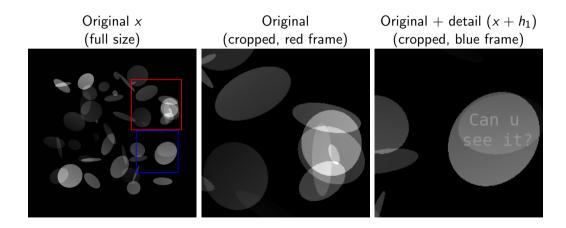
Stable? FIRENETs ✓



Adding FIRENET layers stabilises AUTOMAP

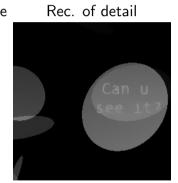


Stability and accuracy, and false negative



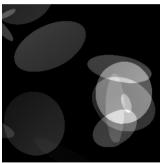
U-net trained without noise

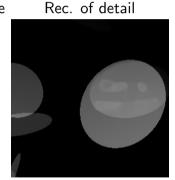
Orig. + worst-case noise Rec. from worst-case noise



U-net trained with noise

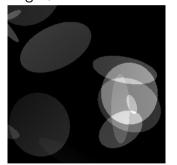
Orig. + worst-case noise Rec. from worst-case noise

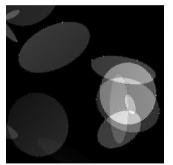




FIRENET

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





Rec. of detail



Concluding remarks

There is a **need for foundations** in AI/deep learning. Our <u>results</u>:

- ► There are well-conditioned problems where mappings from training data to suitable NNs exist, but no training algorithm (even randomised) can approximate them.
- Existence of algorithms depends on desired accuracy. $\forall K \in \mathbb{Z}_{\geq 3}$, \exists well-conditioned problems where simultaneously:
 - (i) Algorithms may compute NNs 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.
- ▶ Under specific conditions, there are algorithms that compute stable NNs. E.g., Fast Iterative REstarted NETworks (FIRENETs) converge exponentially in the number of hidden layers. We prove FIRENETs withstand adversarial attacks.
- There is a trade-off between stability and accuracy in deep learning.

Question: How do we optimally traverse the <u>stability</u> & <u>accuracy</u> trade-off? FIRENETs provide a balance but are likely not the end of the story.

Hopefully this talk has inspired you to build on these results and take up the challenge!