On the Barriers of Deep Learning, Approximate Sharpness, and Smale's 18th Problem

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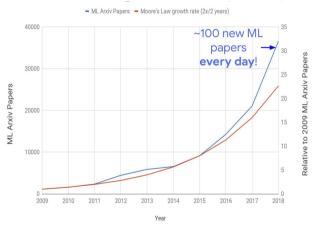
M. Colbrook, V. Antun, A. Hansen, "The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem" (PNAS, to appear) www.github.com/Comp-Foundations-and-Barriers-of-AI/firenet

M. Colbrook, "WARPd: A linearly convergent first-order method for inverse problems with approximate sharpness conditions" (SIIMS, under revision)

www.github.com/MColbrook/WARPd

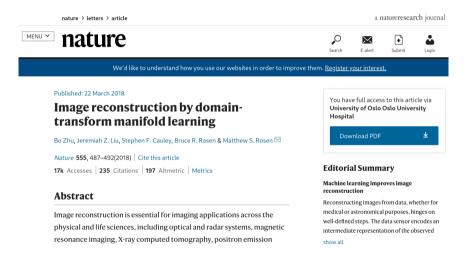
Interest in deep learning unprecedented and exponentially growing

Machine learning papers on arXiv



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

Will AI replace standard algorithms in medical imaging?



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

Very strong confidence in deep learning



Geoffrey Hinton, The New Yorker, April 2017: "They should stop training radiologists now!"

Very strong confidence in deep learning



Geoffrey Hinton, The New Yorker, April 2017: "They should stop training radiologists now!" **BUT** ...

DANGER: Al generated hallucinations Facebook and NYU's 2020 FastMRI challenge

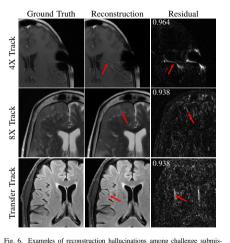
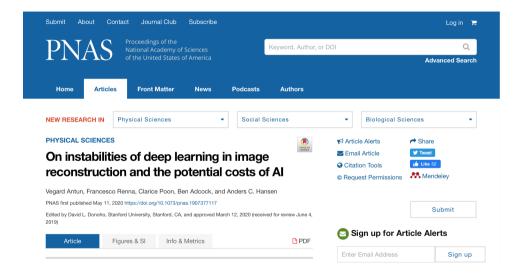
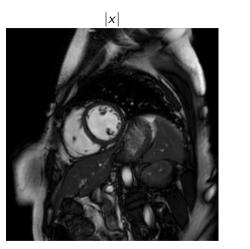
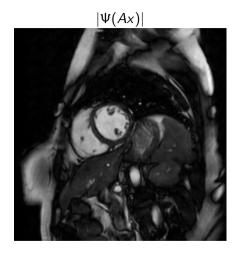


Fig. 6. Examples or reconstruction naturentations among chantenge submissions with SSIM scores over residual plots (residuals magnified by 5). (top) A 4X submission from Neurospin generated a false vessel, possibly related to susceptibilities introduced by surgical staples. (middle) An 8X submission 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.

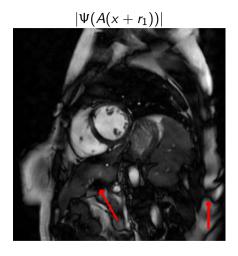
DL seems unstable in inverse problems!

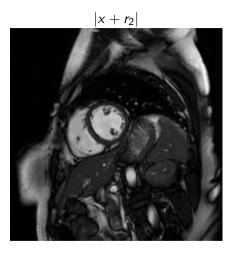


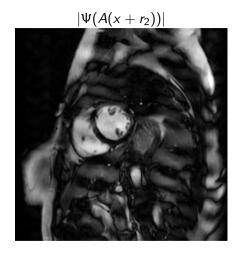




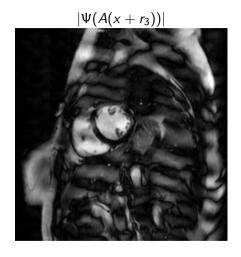




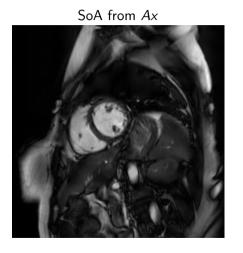


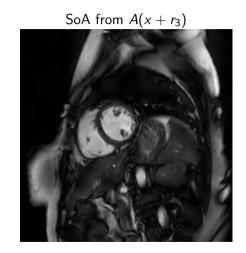






Reconstruction using state-of-the-art standard methods





Optimism: Echoes of an old story

Hilbert's vision (start of 20th century): 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: Provide an algorithm which, for any given polynomial equation with integer coefficients, can decide whether there is an integer-valued solution.

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





Gödel (pioneer of **modern logic**) and Turing (pioneer 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 scientific computation:

- Stability
- Accuracy

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

^{*}Steve Smale's list of problems for the 21st century (requested by Vladimir Arnold), inspired by Hilbert's list $\frac{1}{2}$

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).
- ▶ Some numerical examples (e.g., stability and accuracy).
- Approximate sharpness conditions and Weighted, Accelerated and Restarted Primal-dual (WARPd).

Can we train neural networks that solve (P_i) ?

Sparse regularization (benchmark problem):

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

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

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

Denote the **minimizing** vectors by Ξ .

- \triangleright 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 regularization 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

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

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

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

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 exist a neural network approximating Ξ (solution map of (P_j)), and can it be trained by an algorithm?

(i) **Non-existence:** There does not exist a neural network that approximates the function we are interested in.

(ii)

(iii)

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$$\min_{\mathbf{x} \in \mathbb{C}^N} \|\mathbf{x}\|_{\ell^1}$$
 subject to $\|A\mathbf{x} - \mathbf{y}\|_{\ell^2} \le \eta$ (P₁)

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

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- (i) **Non-existence:** There does not exist a neural network that approximates the function we are interested in.
- (ii) **Non-trainable:** There exists a neural network that approximates the function. However, there does not exist an algorithm that can train the neural network.

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$$\min_{\mathbf{x} \in \mathbb{C}^N} \|\mathbf{x}\|_{\ell^1}$$
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- (i) Non-existence: There does not exist a neural network that approximates the function we are interested in.
- (ii) **Non-trainable:** There exists a neural network that approximates the function. However, there does not exist an algorithm that can train the neural network.
- (iii) **Not practical:** There exists a neural network that approximates the function, and an algorithm training it. However, the algorithm needs prohibitively many samples.

Theorem

For (P_j) , $N \ge 2$ and m < N. Let $K \ge 3$ 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):

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

$$\min_{\substack{y \in \mathcal{S} \ x^* \in \Xi(A,y)}} \inf_{\substack{\phi_{A,\mathcal{S}}(y) = x^* \mid_{\ell^2} \le 10^{-K}, \\ \text{any } n > 1/2}} \|\phi_{A,\mathcal{S}}(y) - x^*\|_{\ell^2} \le 10^{-K}, \quad \forall (A,\mathcal{S}) \in \Omega. \tag{1}$$

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

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

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

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 $\iota_{A,S}$ such that for all $y \in \mathcal{S}$,

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

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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.

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

(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

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

In words ...

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

- ▶ No algorithm, even randomized can train such a neural network accurate to *K* digits with probability greater than 1/2.
- There exists a deterministic algorithm that trains a neural network with K-1 correct digits, but any such (even randomized) algorithm needs arbitrarily many training data.
- ▶ There exists a deterministic algorithm that trains a neural network 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 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

$dist(\Psi_{A_n}(y_n),\Xi_3(A,y))$	$dist(\Phi_{A_n}(y_n),\Xi_3(A,y))$	$ A_n - A \le 2^{-n}$ $ y_n - y _{\ell^2} \le 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	0.000015	n = 10	10^{-6}
0.0000030	0.000015	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.

Can we avoid this?

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

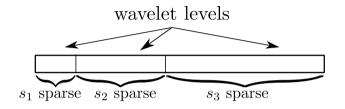
Problem: $f(x) \le f^* + \epsilon$ does not in general imply x is close to set of minimizers.

Question: Can we find 'good' input classes where

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

We shall see that the answer is yes!

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 (s, M)-sparse vectors by $\Sigma_{s, M}$, 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: $f(x) = \lambda ||x||_{\ell^1} + ||Ax - y||_{\ell^2}$

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

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 (s, 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

$$\underbrace{\sigma_{\mathsf{s},\mathsf{M}}(x)_{\ell^1}} + \underbrace{\|Ax - y\|_{\ell^2}}_{} \lesssim \delta, \quad \|x\|_{\ell^2} \lesssim b_1, \quad \|y\|_{\ell^2} \lesssim b_2,$$

distance to sparse in levels vectors noise of measurements

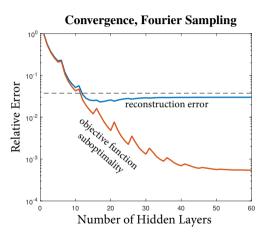
we have the following stable and exponential convergence guarantee in n

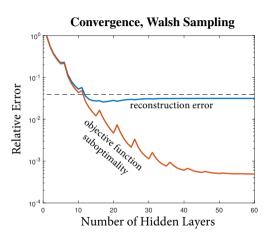
$$\|\phi_n(y)-x\|_{\ell^2}\lesssim \delta+e^{-n}.$$

Demonstration of convergence Image Fourier Sampling Walsh Sampling

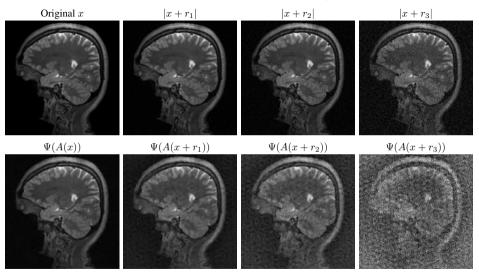
Figure: Images corrupted with 2% Gaussian noise and reconstructed using 15% sampling.

Demonstration of convergence





Stable? AUTOMAP X

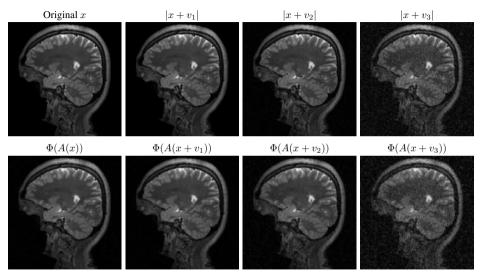


[·] V. Antun et al. "On instabilities of deep learning in image reconstruction and the potential costs of AI," PNAS, 2021.

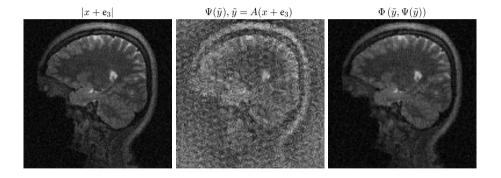
· B. Zhu et al. "Image reconstruction by domain-transform manifold learning," Nature, 2018.

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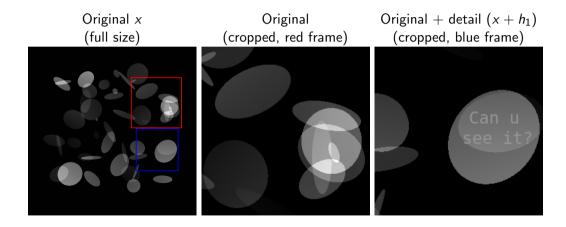
Stable? FIRENETs ✓



Adding FIRENET layers stabilizes AUTOMAP



Stability vs. accuracy tradeoff



U-net trained without noise

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

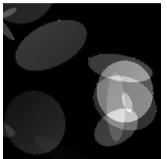
U-net trained with noise

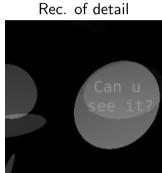
Orig. + worst-case noise Rec. from worst-case noise Rec. of detail

FIRENET

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







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. $\|Ax - y\|_{\ell^2} \le \epsilon$, seminorm \mathcal{J} , $B \in \mathbb{C}^{q \times N}$.

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

Examples: Sparse vector recovery, low-rank matrix recovery, matrix completion (local version holds), 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 $(x,y) \in \mathbb{C}^N \times \mathbb{C}^m$ $\|Ax-y\|_{\ell^2} \leq \epsilon$ and $c(x,y) \leq \delta \Rightarrow \|\phi(y)-x\|_{\ell^2} \lesssim \delta$.

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

Weighted, Accelerated and Restarted Primal-dual (WARPd)

Primal-dual iterations starting at x_0 ($X_k = \text{ergodic average of first } k \text{ iterates}$):

$$\underbrace{\mathcal{J}(X_{k}) + \|BX_{k}\|_{\ell^{1}} - \mathcal{J}(x) - \|BX\|_{\ell^{1}} + C_{2}\left(\|AX_{k} - b\|_{\ell^{2}} - \epsilon\right)}_{=:G(X_{k})} \leq \frac{1}{k} \left(\frac{\|x_{0} - x\|_{\ell^{2}}^{2}}{\tau_{1}} + \frac{C_{2}^{2} + q}{\tau_{2}}\right). \tag{2}$$

- Assumption implies $||X_k x||_{\ell^2} \le C_1(G(X_k) + \delta)$, controls RHS of (2) upon restart.
- \triangleright Reweighting trick and optimize parameters to form map H_k using k (constant) iterations s.t.

$$G(x_0) \leq \alpha_0 \Rightarrow G(H_k(x_0)) \leq \frac{C}{k}(\delta + \alpha_0)$$

Restart iterations when $C/k \le \nu \in (0,1)$ ($\nu = e^{-1}$ optimal). \tilde{X}_p after p restarts: $G(\tilde{X}_p) \le e^{-1}(\delta + e^{-1}(\delta + \dots + e^{-1}(\delta + \alpha_0)) = (e^{-1} + e^{-2} + \dots + e^{-p})\delta + e^{-p}\alpha_0 \le \delta + e^{-p}$.

▶ Apply the assumption to get
$$\|\tilde{X}_p - x\|_{\ell^2} \leq \delta + e^{-p}$$
.

Remarks:

- ► Can be unrolled as a neural network (this inspired the architecture choice for FIRENETS).
 - **NB:** Naive unrolling of PDHG gives slow $\mathcal{O}(\delta + p^{-1})$ convergence.
- Stability (w.r.t. input and execution) can be proven.
- If constants in assumption unknown, can perform grid search at extra logarithmic cost.
- · A. Chambolle, T. Pock, 'A first-order primal-dual algorithm for convex problems with applications to imaging," J
 Math Imaging Vis, 2011.

A final example with different regularizers

A is a DFT, 15% subsampled according to an inverse square law (optimal for TV). Measurements are corrupted with 5% Gaussian noise.

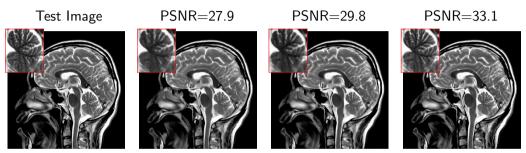


Figure: Middle-left: Converged reconstruction using TV. Middle-right: Converged reconstruction using TGV. Right: Reconstruction using (adaptively adjusted weighted) shearlets and TGV, after 25 iterations. All reconstructions were computed using WARPd.

WARPd can easily handle complicated mixed regularization problems.

$$\min_{\mathbf{x} \in \mathbb{C}^N} \|WD^*\mathbf{x}\|_{\ell^1} + \mathrm{TGV}_{\alpha}^2(\mathbf{x}) \quad \text{s.t.} \quad \|A\mathbf{x} - \mathbf{b}\|_{\ell^2} \le \epsilon,$$

Concluding remarks

There is a **need for foundations** in AI/deep learning.

- Well-conditioned problems where mappings from training data to suitable neural networks exist, but no training algorithm (even randomized) can approximate them.
- ▶ Existence of training algorithms depends on desired accuracy. $\forall K \in \mathbb{Z}_{\geq 3}$, \exists well-conditioned problems where simultaneously:
 - (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.
- ► Under <u>specific conditions</u>, algorithms can train stable and accurate neural networks. E.g., prove **FIRENETs** achieve exponential convergence & withstand adversarial attacks.
- ► There is a <u>trade-off</u> between stability and accuracy in deep learning.
- ▶ WARPd provides accelerated recovery under an approximate sharpness condition.
- Quantities controlling recovery also provide explicit approximate sharpness constants.
- ► WARPd ⇒ motivating architecture choices for FIRENETs.

Question: How do we optimally traverse the stability & accuracy trade-off?