Lipschitz stability of Deep Neural Networks in view of applications

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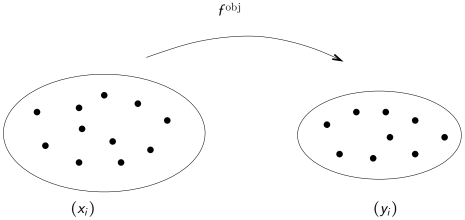
Dataset

- Take a large enough **dataset** : $\mathcal{D} = \{(x_i, y_i),\ i = 1, \ldots\} \subset \mathbb{R}^m \times \mathbb{R}^n$



Postulate : dataset corresponds to unknown objective/transfer function

$$H : \mathbb{R}^m \longrightarrow \mathbb{R}^n$$

with $x_i \in \mathbb{R}^m$, $y_i = H(x_i) + \varepsilon_i \in \mathbb{R}^n$, and noise $\varepsilon_i \in \mathbb{R}^n$.

Least square representation with recursivity

- Take a linear function f with **weight** $W \in \mathcal{M}_{mn}(\mathbb{R})$ and **bias** $b \in \mathbb{R}^n$

$$
\begin{aligned}
f: \quad \mathbb{R}^m &\longrightarrow \mathbb{R}^n, \\
x &\longmapsto f(x) = Wx + b.
\end{aligned}
\tag{1}
$$

- Notations

$a_0 = m$ is the **input layer**

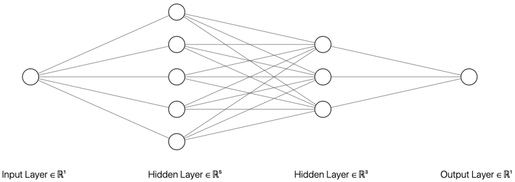
$a_{p+1} = n$ is the **output layer**

$(a_1, a_2, \ldots, a_p) \in \mathbb{N}^p$ are the **(dense) hidden layers** with **neurons**

- Consider

$$
\begin{aligned}
f_r: \quad \mathbb{R}^{a_r} &\longrightarrow \mathbb{R}^{a_{r+1}}, \\
X_r &\longmapsto f_r(X_r) = W_r X_r + b_r
\end{aligned}
$$

and the function $f = f_p \circ f_{p-1} \ldots f_2 \circ f_1 \circ f_0$.



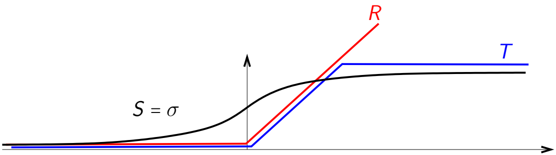
Add non linearity

- Non linearity is added with an **activation function**.

Sigmoid $\in C^1(\mathbb{R})$. A sigmoid σ is monotone, $0 < \sigma' < 1$, with limit value 0 at $-\infty$ and limit value 1 at $+\infty$.

ReLU $\in C^0(\mathbb{R})$. It is defined by $R(x) = \max(0, x)$.
Thresholding yields $T(x) = \min(R(x), 1)$.

Generalization component wise to activation functions $\mathbb{R}^q \to \mathbb{R}^q$.



A function f defined through a generic **feed-forward neural network** is :

$f = f_{p+1} \circ S_{p+1} \circ f_p \circ \cdots \circ f_1 \circ S_1 \circ f_0,$ where activation function is $S_r = \sigma$ or R.

Fit the coefficients with numerical optimisation

Lingo : deep learning=p large, training=numerical optimisation, Machine Learning= optimization, epoch=global iteration, batches=data for local iterations, neural networks=special non linear functions, regression=Least square, ...

- Consider the cost function

$$J(W,b)=\frac{1}{\mathrm{card}\mathcal{D}}\sum_{(x,y)\in\mathcal{D}}|f(x)-y|^2$$

An optimal value satisfies

$$J(W_*,b_*)\le J(W,b)\qquad \forall(W,b).$$

The training=*minimization session on the computer with ad-hoc stochastic gradient algorithms* can extremely difficult since the cost function J is **highly non convex for** $p\ge 2$

- Important variation for classification with CNNs. Let y and $p(z)$ be discrete probabilities : $y_i\in[0,1]$, $\sum y_j=1$; $p_i=\frac{\exp z_i}{\sum_{j=1}^n \exp z_j}\in(0,1)$. Consider the Kullback-Leibler divergence (which is convex)

$$J(W,b)=-\sum_{(x,y)\in\mathcal{D}}(\log p(f(x)),y)\ge 0.$$

What is the stability of the result ?

- Biggio et al : 2013
- Example from Franceshi et al : 2021.

red panda (unperturbed)

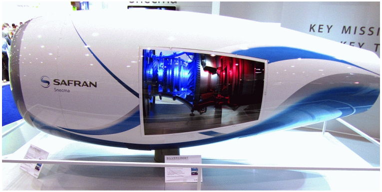
brown bear | teddy bear | polecat | polecat

- Madry et al : Towards deep learning models resistant to adversarial attacks, in 6th International Conference on Learning Representations, 2018.

- Nota Bene : l^1 norm probably better to analyze tables of pixels ≈ images.

A question is :

Can we ***certify*** **with SciML= Scientific Machine Learning these functions/techniques/algorithms/. . . ,**
with critical applications in mind ?



The emerging discipline needs much more on **mathematical stability** of NN functions.

Related ML key words : predictibility, robust IA, control of generalization error, reproductibility, adversarial networks, explainibility, . . .

Model problem

- Assume that f is produce by ML. Consider the dynamical system

$$\begin{cases} x'(t) = f(x(t)), \\ x(0) = x_0 \end{cases}$$

What can we say about the stability of solutions of the ODE ?

- Our model problem is then to :

$\Longrightarrow$ **Evaluate the Lipschitz constant** L

$$|f(x) - f(y)| \leq L|x - y|, \qquad \forall x, y \in \mathbb{R}^n.$$

Setting of the problem

• Take $f : \mathbb{R}^{a_0} \to \mathbb{R}^{a_\ell+1}$

$$f = f_\ell \circ S_\ell \circ f_{\ell-1} \circ S_{\ell-1} \circ \cdots \circ S_1 \circ f_0$$

The regularity is

$$f \in \mathrm{Lip}(\mathbb{R}^{a_0})^{a_{\ell+1}} \subset C^0(\mathbb{R}^{a_0})^{a_{\ell+1}}.$$

Rademacher's Theorem : the gradient is

$$\nabla f(x) = W_\ell D_\ell(x) W_{\ell-1} D_{\ell-1}(x) \dots D_1(x) W_0.$$

A subtlety : use the Murat-Trombetti Theorem (2003) to write down the chain rule formula.

• Take a vectorial norm, for example $\|x\|_{l^p(\mathbb{R}^a)} = \left(\sum_{i=1}^a |x_i|^p\right)^{1/p}$.
The induced norm for matrices is $M \in \mathcal{M}_{ab}(\mathbb{R}) = \mathbb{R}^{a\times b}$ is

$$\|M\| = \|M\|_{l^p(\mathcal{M}_{ab}(\mathbb{R}))} = \max_{x\neq 0} \frac{\|Mx\|_{l^p(\mathbb{R}^a)}}{\|x\|_{l^p(\mathbb{R}^b)}}. \quad (2)$$

• Our goal is to obtain sharp upper bounds on

$$L = \sup_{x\in\mathbb{R}^{a_0}} \|\nabla f(x)\|_{l^p\left(\mathcal{M}_{a_{\ell+1},a_0}(\mathbb{R})\right)} = \left(\|\nabla f\|_{l^p\left(\mathcal{M}_{a_{\ell+1},a_0}(\mathbb{R})\right)}\right)_{L^\infty(\mathbb{R}^{a_0})}.$$

Previous results (all in L^2 norms as far we understand)

• Everywhere. One has $L \leq K_\star$ where $K_\star = \prod_{r=0}^{\ell} \| W_r \|$.

• Szegedy et al (2013). On has $L \leq K \leq K_\star$ where

$$K = \max_{D \in \mathcal{D}} \| W_\ell D_\ell W_{\ell-1} D_{\ell-1} \dots D_1 W_0 \|,$$

Note immediately the complexity $2^{a_0 + a_1 + \cdots + a_\ell} = \Pi_{r=0}^{\ell} 2^{a_r}$.

• Virmaux-Scaman (2019). Find upper bound on K with SVD decomposition. The complexity reduces to $\sum_{r=0}^{\ell} 2^{a_r}$.

• Combettes-Pesquet (2020). Define $W_{(t,s)} = W_{t-1} W_{t-2} \dots W_{s+1} W_s$. Then $K \leq K_1 \leq K_\star$ where

$$K_1 = \frac{1}{2^\ell} \sum_{1 \leq r_1 < r_2 < \cdots < r_n \leq \ell} \| W_{(\ell+1, r_n)} \| \| W_{(r_n, r_{n-1})} \| \dots \| W_{(r_2, r_1)} \| \| W_{(r_1, 0)} \|.$$

The complexity is $2^\ell \ll \sum_{r=0}^{\ell} 2^{a_r} \ll \Pi_{r=0}^{\ell} 2^{a_r}$.

Simple proof of C.P.

Define $Z_r = 2D_r - I_r = \mathrm{diag}(\pm 1)$ so that $D_r = \frac{1}{2}(I_r + Z_r)$.
Define $\mathcal{Z}_r = \{Z_r\}$ and $\mathcal{Z} = \mathcal{Z}_\ell \times \cdots \times \mathcal{Z}_1$.

$$
\begin{aligned}
K &= \max_{D\in\mathcal{D}} \| W_\ell D_\ell W_{\ell-1} D_{\ell-1} \dots D_1 W_0 \| \\
&= \max_{Z\in\mathcal{Z}} \left\| W_\ell \left(\frac{1}{2}(I_\ell + Z_\ell)\right) W_{\ell-1} \left(\frac{1}{2}(I_{\ell-1} + Z_{\ell-1})\right) \dots \left(\frac{1}{2}(I_1 + Z_1)\right) W_0 \right\| \\
&\le \frac{1}{2^\ell} \max_{Z\in\mathcal{Z}} \sum_{1\le r_1 < r_2 < \dots < r_n \le \ell} \| W_{(\ell+1,r_n)} Z_{r_n} W_{(r_n,r_{n-1})} \dots W_{(r_2,r_1)} Z_{r_1} W_{(r_1,0)} \| \\
&\le \frac{1}{2^\ell} \max_{Z\in\mathcal{Z}} \sum_{1\le r_1 < r_2 < \dots < r_n \le \ell} \| W_{(\ell+1,r_n)} \| \| Z_{r_n} \| \| W_{(r_n,r_{n-1})} \| \dots \| W_{(r_2,r_1)} \| \| Z_{r_1} \| \| W_{(r_1,0)} \| \\
&\le \frac{1}{2^\ell} \sum_{1\le r_1 < r_2 < \dots < r_n \le \ell} \| W_{(\ell+1,r_n)} \| \| W_{(r_n,r_{n-1})} \| \dots \| W_{(r_2,r_1)} \| \| W_{(r_1,0)} \| \\
&= K_1 \le K_\star .
\end{aligned}
$$

"Trivially", one also $K \le K_\star$.

A first new bound

It is well known that
$\|A\|_1 = \max_{1\le j\le n} \sum_{i=1}^{m} |A_{ij}|$ and $\|A\|_\infty = \max_{1\le i\le m} \sum_{j=1}^{n} |A_{ij}|$.

Definition

Given a matrix $A \in \mathcal{M}_{m,n}(\mathbb{R})$, denote $A^{\mathrm{abs}} \in \mathcal{M}_{m,n}(\mathbb{R})$ the matrix such that

$$(A^{\mathrm{abs}})_{ij} = |A_{ij}|, \qquad \forall i, j.$$

One obtains
$\|A\|_1 = \|A^{\mathrm{abs}}\|_1$ and $\|A\|_\infty = \|A^{\mathrm{abs}}\|_\infty$ (not true for l^2-based norms).

Theorem

One has the bound $K \le K_3$ where

$$K_3 = \|W_\ell^{\mathrm{abs}} W_{\ell-1}^{\mathrm{abs}} \dots W_0^{\mathrm{abs}}\|_{1,\infty}.$$

Combine with the Combettes-Pesquet trick

$$K_4 = \frac{1}{2^\ell} \sum_{1 \le r_1 < r_2 < \cdots < r_n \le \ell} \| W^{\mathrm{abs}}_{(\ell+1, r_n)} \ldots W^{\mathrm{abs}}_{(r_2, r_1)} W^{\mathrm{abs}}_{(r_1, 0)} \|_{1,\infty}.$$

Theorem

One has the bounds $K \le K_4 \le K_1$.

Summary of these bounds

Here we use l^1 and l^∞ norms

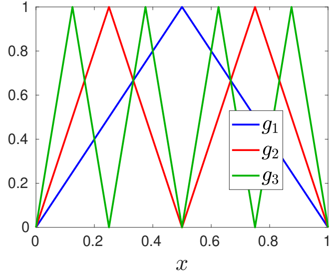
$$L \leq K \leq K_4 \leq \min(K_1, K_3) \leq \max(K_1, K_3) \leq K_\star.$$

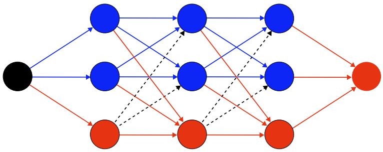
Approximation of x^2

$$g(x) = \begin{cases} 2x, & x \in [0, 0.5) \\ 2(1-x), & x \in [0.5, 1] \end{cases}, \quad g_r(x) = \underbrace{g \circ g \circ \cdots \circ g \circ g}_{r \text{ times}}.$$

Converging series : Takagi (1902), Yarostky (2017), Devore et al, D., ...

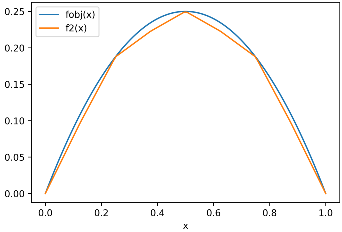
$$x^2 = x - \sum_{r=0}^{\infty} \frac{g_r(x)}{4^r}.$$



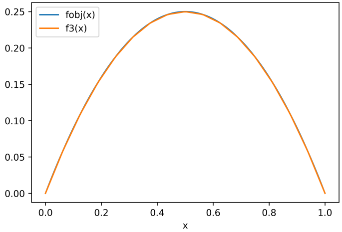


Graphical representation of the truncated network $x - \sum_{r=0}^{3} \frac{g_r(x)}{4^r}$.

Illustration : $x \mapsto x - x^2$



two layers



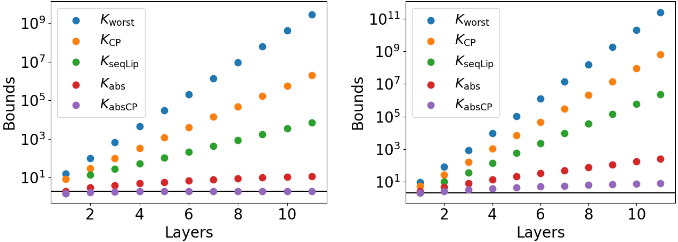
three layers

Clearly $\left\| x^2 - \left(x - \sum_{r=1}^{p} \frac{1}{4^r} g_r(x)\right)\right\|_{L^\infty(0,1)} \leq \sum_{p+1\leq n} \frac{1}{4^r} = \frac{1}{3\times 4^p}$.
Width $N = 3$, depth p : accuracy is $\varepsilon = O(4^{-p})$, for a cost Cost $= O(3\times p) \approx C|\log\varepsilon|$.

Theorem (Yarostky 2017)

There exists a NN approximating all bounded functions $\in W^{n,\infty}([0,1]^d)$ with uniform accuracy ε, uniform cost $\approx \log 1/\varepsilon$ and at most $\approx \varepsilon^{-d/n}\log 1/\varepsilon$ computational units.

Results and optimality of K_4



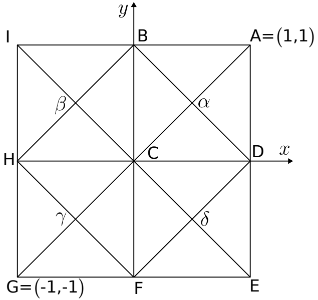
Bounds depending on the ReLU representation of g.

ℓ	L	K_*	K_1	K_2	K_3	K_4
1	1.5	3.0	2.0	1.5	2.0	1.5
2	1.75	9.0	3.53125	3.64531	3.0	1.75
3	1.875	33.0	6.92187	6.45925	4.0	1.875
4	1.93875	129.0	14.42877	12.45882	5.0	1.93875
5	1.96875	513.0	30.75637	24.68184	6.0	1.96875
6	1.984375	2049.0	66.00227	49.24501	7.0	1.984375

A test for $T(x,y) = xy$

A new formula with strong connexion with FEM : consider the function

$$\Lambda = (\Lambda_1, \Lambda_2) : \mathbb{R}^2 \to \mathbb{R}^2$$



$$\Lambda_1 = \varphi_\alpha - \varphi_\beta + \varphi_\gamma - \varphi_\delta$$
$$\Lambda_2 = \varphi_D - \varphi_A + \varphi_B - \varphi_C + \varphi_F - \varphi_E - \varphi_G + \varphi_H - \varphi_I,$$

Formula

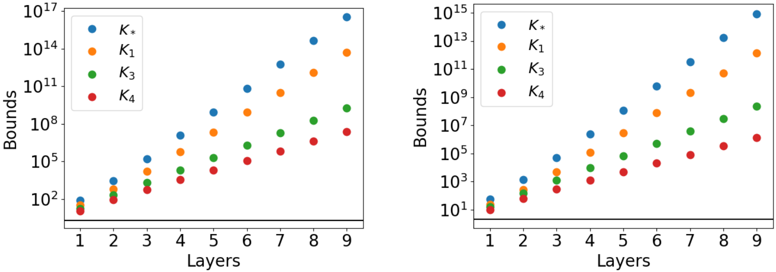
One can check the formula where $e_0 \in P^1_{\mathrm{FEM}}$

$$T = e_0 + \frac{1}{4} T \circ \Lambda \Longrightarrow T = \sum_{n \geq 0} \frac{1}{4^n} e_0 \circ \underbrace{\Lambda \circ \cdots \circ \Lambda}_{n \text{ times}}.$$

It reveals the power of composition.

Results

Lipschitz bounds for networks approximating the function xy.



Remark : the formula is an alternative to the multiplyer function in the influental contribution Yarotsky 2017.

Matrices with random weights (from C.P.)

Take $W_3 \in \mathcal{M}_{3,6}(\mathbb{R})$, $W_2 \in \mathcal{M}_{6,10}(\mathbb{R})$ and $W_1 \in \mathcal{M}_{10,8}(\mathbb{R})$. Their entries are i.i.d. realizations of the normal distribution $\mathcal{N}(0,1)$.

$$f = f_3 \circ R \circ f_2 \circ R \circ f_1, \qquad R = \text{ReLU}.$$

Statistic	K/K_*	K_1/K_*	K_2/K_*	K_3/K_*	K_4/K_*
Maximum	0.2772	0.5786	0.6789	0.8023	0.4608
Average	0.1422	0.4539	0.3256	0.5461	0.2875
Minimum	0.0595	0.3703	0.1597	0.2897	0.1604
Standard deviation	0.0343	0.0350	0.0685	0.0813	0.0483

Statistics over 1000 realizations.

Once again, K_4 is the best one.

Convolutional neural networks

CNNs are central for classification, as exemplified by the MNIST dataset

$$g = T_{\ell+1} \circ g_\ell \circ T_\ell \circ g_{\ell-1} \circ T_{\ell-1} \circ \cdots \circ T_1 \circ g_0.$$

For simplification we neutralize the last soft-max function $T_{\ell+1} = I$.

$$g = g_\ell \circ T_\ell \circ g_{\ell-1} \circ T_{\ell-1} \circ \cdots \circ T_1 \circ g_0.$$

Normalization is that g_r have ability to change the dimension and that the T_r do not change the dimension.

As before, a linear function $g_i^{\mathrm{lin}} : \mathbb{R}^{a_i} \to \mathbb{R}^{a_{i+1}}$ is written

$$g_i^{\mathrm{lin}}(x) = W_i x + b_i.$$

Convolutional layers

- A convolutional layer $g_i^{\text{con}} : \mathbb{R}^{a_i} \to \mathbb{R}^{a_{i+1}}$

$$g_i^{\text{conv}}(x) = K_i^{\text{conv}} * \overline{x} + \overline{b}_i.$$

Since convolution operators are linear operators, there exist a matrix $W_i = W_i^{\text{conv}}$ such that

$$g_i^{\text{conv}}(x) = W_i x + b_i,$$

Example : take a vertical vector

$$x = \begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{21} & x_{22} & x_{23} & x_{31} & x_{32} & x_{33} \end{bmatrix}^T \in \mathbb{R}^9. \tag{3}$$

A re-indexation allows to write

$$\overline{x} = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{bmatrix} \tag{4}$$

- The normalization convention allows to represent the non-linear **max-pool function** as a g_i

$$g_i(x) = (\max(x_{11}, x_{12}, x_{21}, x_{22}), \dots) \in \mathbb{R}^4.$$

$$g \in \mathrm{Lip}(\mathbb{R}^{a_0})^{a_{\ell+1}} \subset C^0(\mathbb{R}^{a_0})^{a_{\ell+1}}.$$

All previous results are generalized mutatis mutandi.

A test with CNN (MNIST, LeCun et al)

Introduction

Lipschitz stability

Extension to CNN

Training with regularization (0.01).
The accuracy on the test set is always between 95% and 97%.

Model	Approach	l^1				l^∞			
		K_*	K_1	K_3	K_4	K_*	K_1	K_3	K_4
Model A	Explicit	1.058e5	1.107e4	9.377e3	2.222e3	1.565e6	1.734e5	2.993e5	4.756e4
	Implicit	1.562e2	4.721e1	5.191e1	**2.739e1**	3.678e3	9.021e2	1.859e3	**6.424e2**
Model B	Explicit	1.712e7	7.353e5	1.599e5	3.626e4	2.878e7	3.171e6	4.590e6	6.804e5
	Implicit	4.280e2	1.423e2	1.772e2	**1.016e2**	1.151e4	2.823e3	6.203e3	**2.294e3**
Model C	Explicit	4.950e8	1.910e7	3.120e6	7.327e5	8.241e8	7.749e7	9.068e7	1.170e7
	Implicit	7.735e2	2.337e2	1.853e2	**1.230e2**	2.060e4	4.570e3	6.574e3	**2.307e3**

Once again, K_4 is the best one.

Conclusion

- Stability of NNs is a fundamental topic, at least for the development of SciML and potential applications to certification.
- Linear algebra has something to say about the Lipschitz stability of NNs. So far K_4 is systematically the best estimate.
- **Open question 1 :** find better bounds through spectral analysis.
- **Open question 2 :** use such bounds to regularize training.
- **Open question 3 :** use such bounds for applications such as "learning real problems" and "solving PDEs".

D.-Pintore : Certified computable Lipschitz bounds for Deep Neural Networks.