Provable approximations on smooth manifolds using deep neural networks

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Outline

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Function classes of Neural Networks

Neural networks produce **structured parametric families of functions** of the form

$$\Phi(x) = W_L \circ \rho \circ W_{L-1} \circ \dots \rho \circ W_1(x), \quad x \in \mathbb{R}^D$$

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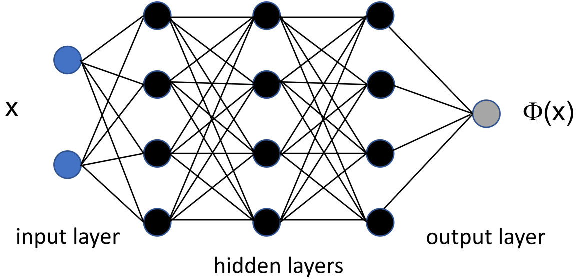
where

- $W_\ell(x) = A_\ell x + b_\ell, \quad \ell = 1, \ldots, L$
- $A_\ell \in \mathbb{R}^{N_\ell \times N_{\ell-1}}$ are the **filters** and $b_\ell \in \mathbb{R}^{N_\ell}$ are the **biases**
- $\rho : \mathbb{R} \to \mathbb{R}$ is the **activation function**
- $L(\Phi)$ is the **number of layers** of Φ
- $N_\ell \in \mathbb{N}$, $i = \ell, \ldots, L$ is the **width** of the ℓ-th layer, $N_0 = D$, and $N(\Phi) = \sum_{i=0}^{L} N_i$ is the **number of neurons** of Φ
- $M(\Phi) = \sum_{\ell=1}^{L} ||A_\ell||_0 + ||b_\ell||_0$ is the **number of weights** (or **parameters**) of Φ

Function classes of Neural Networks

Graph representation



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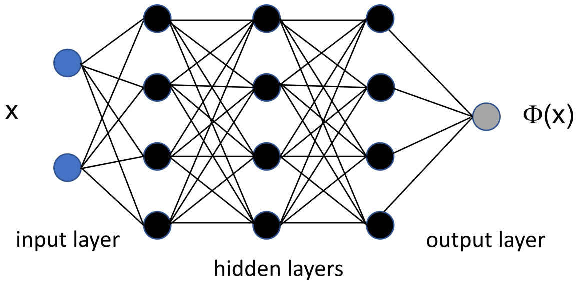

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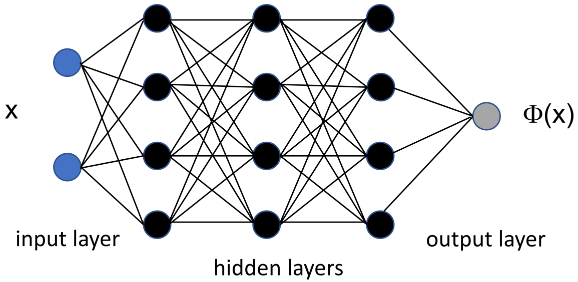

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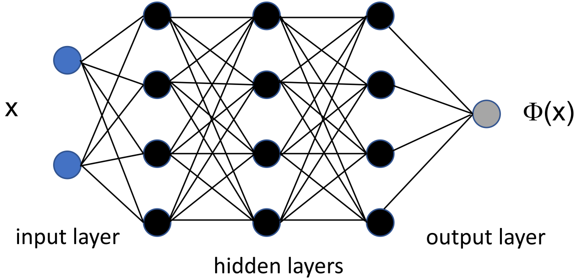

- Number of layers $L = 4$
- Number of neurons $N = 15$
- Number of weights $M = \sum_{\ell=1}^{4} ||A_\ell||_0 + ||b_\ell||_0 = 44 + 12 = 56$

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Assumption: I wil identify a neural network with the **function** implemented by the neural network

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Definition

For a tuple (M_0, L_0, B_0), where $M_0, L_0 \in \mathbb{N} \cup \{\infty\}$ and $B_0 > 0$, $\mathcal{F}(M_0, L_0, B_0)$ denotes the **function class** of neural networks with number of weights M_0, number of layers L_0 and with scale B_0:

$$\mathcal{F}(M_0, L_0, B_0) = \left\{ \Phi \colon [0,1]^D \to \mathbb{R}^{N_L} \,\middle|\, L(\Phi) \leq L_0, W(\Phi) \leq W_0, B(\Phi) \leq B_0 \right\}$$

where $B(\Phi) = \max_\ell \{||vec(A_\ell)||_\infty, ||b_\ell||_\infty\}$ is the **scale** of the weights of Φ

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Examples of activation functions:

- **Sigmoid**: $\rho(x) = \frac{1}{1+e^{-x}}$
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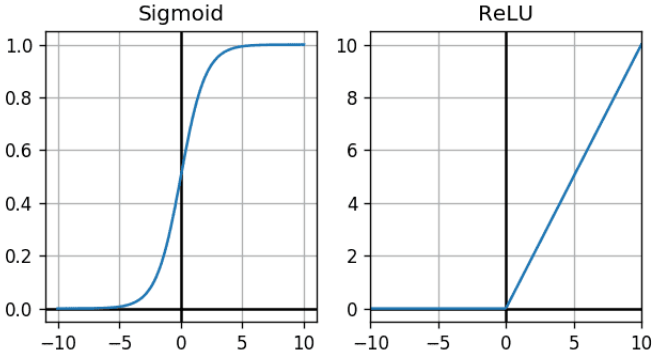

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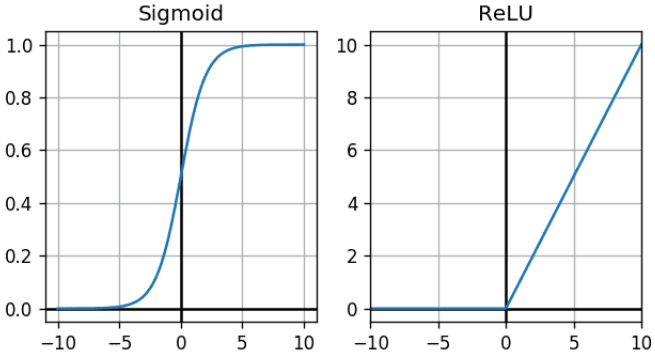

- ReLU is most commonly used in applications

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Theorem [Cybenko, 1989]

Assume ρ is a sigmoidal activation function.
For every $f \in C([0,1]^D)$, given $\varepsilon > 0$, there exists $\Phi \in \mathcal{F}(M, L = 2, B)$, such that

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Note: number of weights $M(\Phi)$ ($\Rightarrow$ number of neurons $N_2(\Phi)$) can become arbitrarily large.

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  - The functions $\rho(ax + b)$ belong to $\Phi \in \mathcal{F}(M, L = 2, B)$ for any $a \in \mathbb{R}^D$, $b \in \mathbb{R}$.
  - Contradiction follows since ρ is **discriminatory**, i.e., the only Radom measure μ for which $\int_{[0,1]^D} \rho(ax + b)\, d\mu(x) = 0$, $a \in \mathbb{R}^D$, $b \in \mathbb{R}$, is the zero measure.

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Theorem [Kidger and Lyons, 2020]

Assume ρ is a nonaffine continuous function which is continuously differentiable at least one point, with nonzero derivative at that point. For every $f \in C([0,1]^D)$, given $\varepsilon > 0$, there exists a neural network $\Phi : \mathbb{R}^D \to \mathbb{R}^d$ where the number of neurons N_ℓ for each layer ℓ bounded by $D + d + 2$ such that

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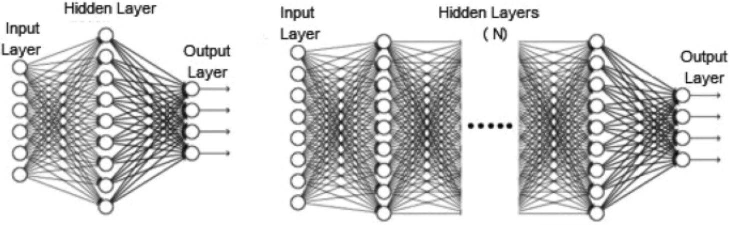
Note: number of layers $L(\Phi)$ can become arbitrarily large.

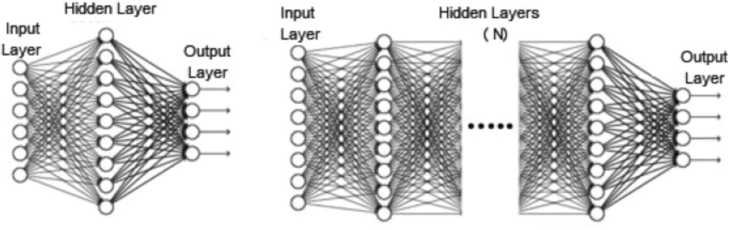
Deep Neural Networks



(a) A Shallow Network (b) A Deep Neural Network

- Modern network architectures are typically very deep

Deep Neural Networks



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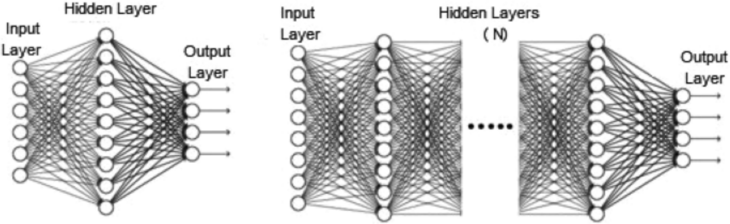

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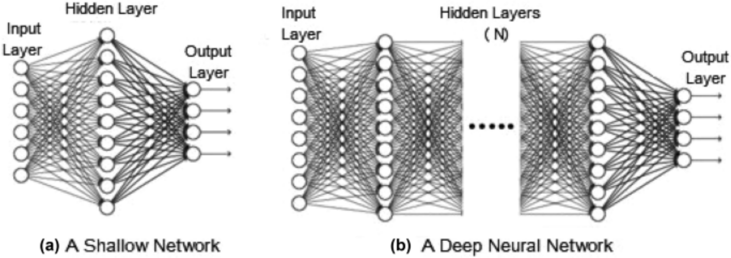

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- **Deep** vs. **shallow networks**: Depth improves expressive power
- With respect to shallow networks (and traditional function representations), deep neural networks can exploit **composition** → **Blessing of compositionality**

Example: piecewise linear functions on $\mathbb{R}$

Triangle function:

$$T(x) = \begin{cases} 2x & \text{if } 0 \le x < \frac{1}{2} \\ 2(1-x) & \text{if } \frac{1}{2} \le x \le 1 \end{cases} \qquad x \in \mathbb{R},$$

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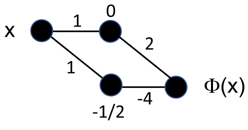

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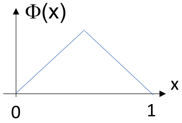

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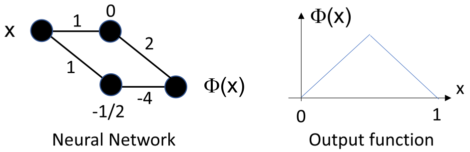

- $\Phi(x)$ is a neural network with $L = 2$, $N_2 = 2$, $M = 6$.

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- Deep neural networks can **improve classical approximation methods** for several function classes
  [Daubechies, DeVore, Foucart, Hanin, Petrova, 2022]

Approximations using Neural Networks

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Consider $f \in C([0,1]^D)$. Then

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Let f be piecewise $C^\beta([0,1]^D)$ with $\beta > 0$. Then

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- The constant c depends on D, β but dependence is not explicit

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[Lu, Shen, Yang, Zhang, 2020], [Shen, Yang, Zhang, 2021] are the first papers to provide **non-asymptotic** and **quantitative** approximation results.

Approximations using Deep Neural Networks

Theorem [Shen, Yang, Zhang, 2021]

Let $f \in B_\lambda(C^\alpha([0,1]^D))$, the space of Hölder continuous function of order $\alpha \in [0,1)$ with Hölder constant λ, and let $\mathcal{F}(N,L,B)$ where N is the width and L is the depth of Φ
Then, for $p \in [1,\infty]$

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Outline...

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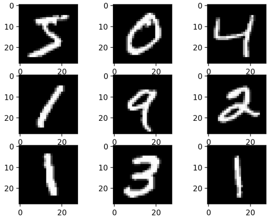

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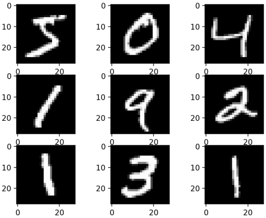

- ImageNet: $224 \times 224 \times 3 = 150528$ pixels per image $\to \mathbb{R}^{150528}$
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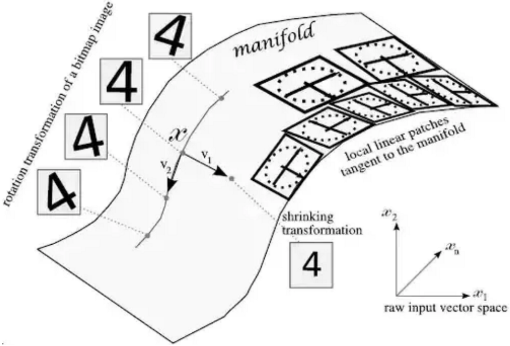
Manifold hypothesis

Many theoretical results explains this phenomenon either explicitly or implicitly using the manifold hypothesis.

Manifold hypothesis:

There is a d-dimensional manifold containing our D-dimensional data of interest where $d \ll D$



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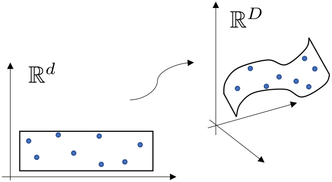

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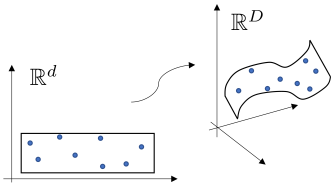

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Bonus: neural networks can learn local coordinate transformations

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[Shaham,Cloninger,Coifman,2018; Schmidt-Hieber,2019; Nakada,Imaizumi,2020]

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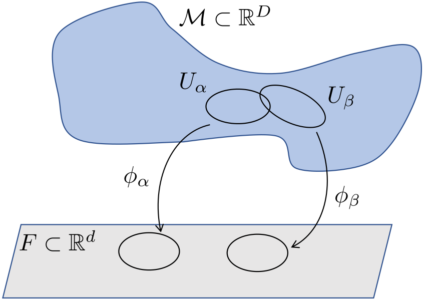

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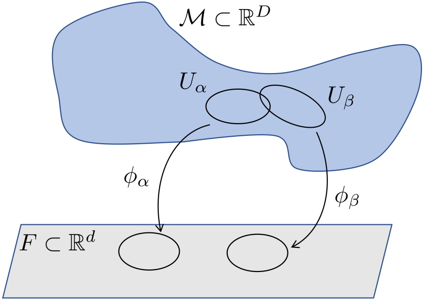

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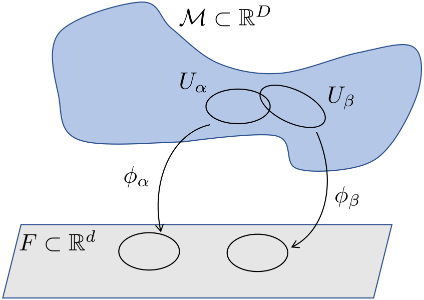

4. Extend the basis or frame terms from the original domain on $\mathbb{R}^d$ to $\mathbb{R}^D$ in a way that depends on the curvature of the manifold.

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Our result [Labate,Shi, 2022]

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- Recent application in the context of approximations using neural networks: [Cai, Li, Sun, Wang, 2019], [Shen, Yang, Zhang, 2021]

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Theorem [Baraniuk and Wakin, 2009]

Let $\mathcal{M} \subset \mathbb{R}^D$ be a compact d-dimensional Riemannian submanifold having condition number $1/\tau$, volume V, and geodesic covering regularity $\mathcal{R}$. Fix $\delta, \gamma \in (0,1)$ and let A be a random orthoprojector from $\mathbb{R}^D$ to $\mathbb{R}^{d_\delta}$ with

$$d_\delta = \mathcal{O}\left(\frac{d \log(DV\mathcal{R}\tau^{-1}\delta^{-1})}{\delta^2}\right) = \mathcal{O}\left(d\frac{\log(D\delta^{-1})}{\delta^2}\right)$$

Then, for every pair of points $x_1, x_2 \in \mathcal{M}$

$$(1-\delta)\sqrt{\frac{d_\delta}{D}}\,|x_1 - x_2| \le |Ax_1 - Ax_2| \le (1+\delta)\sqrt{\frac{d_\delta}{D}}\,|x_1 - x_2|$$

holds with probability at least $1-\gamma$.

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4. By applying the mapping A, derive from $\Phi^{\tilde{g}_0}$ a neural network Φ^{f_0} to approximate f_0 on $\mathcal{M}$

Challenges:

Network approximation - Manifold hypothesis

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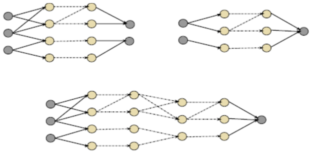
Concatenation. Given neural networks $\Phi_1 \in \mathcal{F}(M_1, L_1, B_1)$ and $\Phi_2 \in \mathcal{F}(M_2, L_2, B_2)$, the concatenation of Φ_1 and Φ_2 is another neural network $\Phi_1 \circ \Phi_2 \in \mathcal{F}(2M_1 + 2M_2, L_1 + L_2 - 1, \max(B_1, B_2))$



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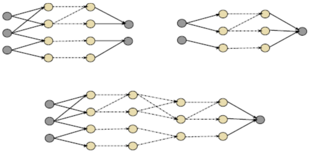

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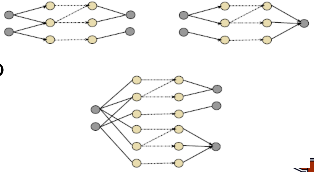

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Idea of the proof: 1-2. Approximation of $B_\lambda(C^\alpha([0,1]^D))$

Proposition (Approximation of monomials). Fix $b > 0$ and $D \in \mathbb{N}$. For any $\varepsilon > 0$ and $\nu \in \mathbb{N}^D$ with $|\nu| \leq b$ there is a neural network $\Phi_\varepsilon^{\mathrm{mul}} \in \mathcal{F}(M, L, B)$ with D-dimensional input and 1-dimensional output satisfying

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We can choose $M = N(\Phi_\varepsilon^{\mathrm{mul}})$, $L = L(\Phi_\varepsilon^{\mathrm{mul}})$, $B = B(\Phi_\varepsilon^{\mathrm{mul}})$ such that

- $W \le 384\, 6^D\, b \left(119 + 36\lfloor 1/D \rfloor + (384)\, 4^{\lfloor 1/D \rfloor}\right) \varepsilon^{-D}$,
- $L \le (1 + \lceil \log_2 \lfloor b \rfloor \rceil)(11 + 1/D)$,
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Proof. Refinement of result in [Petersen and Voigtlaender, 2018].

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g is not guaranteed to be Hölder continuous but can be approximated uniformly with small error by a function $\tilde{g} \in B_{\tilde{\lambda}}(C^\alpha([0,1]^{d_\delta}))$
By concatenation we can define an approximating neural network, $\Phi^f = \Phi^{\widetilde{g}} \odot ((A, 0))$ giving

$$|g(y) - \Phi^f(x)| \leq |g(y) - \tilde{g}(y)| + |\tilde{g}(Ax) - \Phi^{\tilde{g}}(Ax)|$$

Application: Generalization error

We show an application of the approximation result to the problem of controlling the **generalization error** in a regression problem.

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where

- $f_0 \in B_\lambda(C^\alpha([0,1]^D))$,
- the covariates X_i marginally follow a probability measure μ,
- the errors ε_i are i.i.d normally distributed with mean 0 and variance σ^2 and are independent of the X_i.

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To estimate the regression function f_0, we compute the least square estimator $\widehat{\Phi} \in \mathcal{F}(M, L, B)$ of f_0 associated with the **empirical risk minimization**

$$\widehat{\Phi} = \underset{\substack{\Phi = g \circ A \\ g \in \mathcal{F}(M,L,B)}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \big(Y_i - \Phi(X_i)\big)^2 ,$$

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with the estimator returning a neural network $\widehat{\Phi}$ of the form $g \circ A$ where $g \in \mathcal{F}(M, L, B)$ and A is a random orthoprojection

$$A : \mathbb{R}^D \to \mathbb{R}^{d_\delta} \quad d < d_\delta < D$$

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Theorem (informal version)

Let $\mathcal{M} \subset \mathbb{R}^D$ be a Riemannian d-dimensional manifold (with some regularity) and let $f \in B_\lambda(C^\alpha([0,1]^D))$, $\alpha \in (0,1)$. Let $\widehat{\Phi}$ be the solution of the empirical risk minimization problem given above. Then there exists a constant $c = c(\sigma, \beta, d_\delta, \lambda)$ such that

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- Complexity of the network depends weakly on D. M depends linearly with D and L, B do not depend on D but only on d_δ.

Outline...

Conclusion

- Application of Johnson-Lindenstrauss lemma is useful to manage COD using neural networks without the need to define an explicit atlas from the ambient space $\mathbb{R}^D$ into the lower dimensional space $\mathbb{R}^d$ and improved control over the dependence of the parametrization of the network on D.

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- The drawback is that this approach offers limited control over the regularity of f
- How to adapt this approach to smooth and piecewise smooth functions such as Hölder function with smoothness $\alpha > 1$ and Besov spaces?

Questions?

References + codes at: `www.math.uh.edu\~dlabate`