

# Linear and Nonlinear Schemes for Forward Model Reduction and Inverse Problems

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- 1 Elements of approximation theory
  - Linear and Nonlinear Approximation
  - Nonlinear approximation with Neural Networks
- 2 Forward Problem: Reduced Order Modelling of parametrized PDEs
  - Linear and Nonlinear MOR
  - Role of geometry
- 3 Inverse Problems
  - Optimal linear and nonlinear algorithms for State Estimation
  - Role of Geometry
- 4 Hands-on session with Agustin Somacal



- Slides: [www.olgamula.com](http://www.olgamula.com)
- Notebook:



<https://github.com/agussomacal/ROMHighContrast/tree/NonLinearROM>

- **Lecture Notes: Inverse Problems: A Deterministic Approach using Physics-Based Reduced Models, OM.**

**Part I.1**  
**Elements of approximation theory**  
**Linear and Nonlinear Approximation**

Let  $(V, \|\cdot\|)$  be a Banach/Hilbert space.

Examples:  $V = \mathbb{R}^d, L^p(\Omega), W^{k,p}(\Omega)$ , with  $\Omega \subset \mathbb{R}^d$ .

The goal of approximation is to **replace** a target function  $u \in V$  by a simpler function (easy to work with in practice).

An approximation is searched in a set of functions  $V_n \subset V$ , where  $n$  is related to some **complexity** measure, typically the number of parameters.

We distinguish:

- **linear approximation** when  $V_n$  is a finite-dimensional linear space

$$V_n = \text{span}\{v_i\}_{i=1}^n = \left\{ \sum_{i=1}^n c_i v_i : c_i \in \mathbb{R} \right\}$$

where the  $\{v_i\}_{i=1}^n$  form a basis of  $V_n$ .

Examples of  $v_i$ : polynomials, trigo. polynomial, fixed knot splines...

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- **nonlinear approximation** when  $V_n$  is a nonlinear set. Examples:
  - $n$ -term approximation

$$V_n = \left\{ \sum_{i=1}^n c_i v_i : c_i \in \mathbb{R}, v_i \in \mathcal{D} \right\}$$

where  $\mathcal{D} = \{v_i\}_{i=1}^\infty$  is a dictionary of functions

Examples: rational functions, free-knot splines, neural networks, tensor networks...

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- **nonlinear parametric manifold:**

$$V_n = \{D(c) : c \in \mathbb{R}^n\}$$

with some given nonlinear map  $D : \mathbb{R}^n \rightarrow V$ .

Examples: rational functions, free-knot splines, neural networks, tensor networks...

We take the view that nonlinear approximation methods depending on  $n$  parameters are built on two mappings:

- An **encoder** mapping

$$E : V \rightarrow \mathbb{R}^n$$

which when given  $u \in V$  chooses  $n$  parameters  $E(u) \in \mathbb{R}^n$  to represent  $u$ .

- A **decoder** mapping

$$D : \mathbb{R}^n \rightarrow V$$

which maps a vector  $c \in \mathbb{R}^n$  back into  $V$  and is used to build the approximation of  $u$ .

The set

$$V_n := \text{Im}(D) = \{D(c) : c \in \mathbb{R}^n\} \subset V$$

is viewed as a **parametric manifold**.

**Remark:** The encoder-decoder scheme describes a process of dimensionality reduction.

- **Linear orthogonal projection:**

- $V$  Hilbert,  $V_n = \text{span}\{v_i\}_{i=1}^n$ ,  $\{v_i\}$  ONB
- Choose  $E(u) = (\langle u, v_i \rangle)_{i=1}^n$ .
- Choose  $D(c) = \sum_{i=1}^n c_i v_i \in V_n$
- $u \approx D(E(u)) = \sum_{i=1}^n \langle u, v_i \rangle v_i = P_{V_n} u$

- **Compressed sensing:**

- $V = \mathbb{R}^N$  with  $N \gg 1$ .
- $\Sigma_k^N$ : Vectors of  $\mathbb{R}^N$  with at most  $k$  non zero entries.
- Task: Approximate  $u \in \Sigma_k^N$  from  $m$  observations  $\Phi_1^T u, \dots, \Phi_m^T u$  (with  $1 \leq m \leq N$ ).
- Choose  $E(u) = \Phi^T u$  with  $\Phi = [\Phi_1 | \dots | \Phi_m]$
- Choose  $D(c) = \arg \min_{v \in \mathbb{R}^N} \{\|v\|_{\ell_1} : \Phi^T v = c\} \in \Sigma_k^N$
- $u \approx D(E(u)) \in \Sigma_k^N$

- **Neural Networks** (see later on).

Let  $(V, \|\cdot\|)$  be a normed space,  $V_n$  a given approximation set.

For a given target function  $u \in V$ , the error of **best approximation**

$$e_n(u) = \inf_{v \in V_n} \|u - v\|$$

quantifies the best we can expect from  $V_n$ .

For a sequence  $(V_n)_{n \geq 1}$  of sets of growing complexity:

- **(universality)** Does  $e_n(u) \rightarrow 0$  as  $n \rightarrow \infty$  for all  $u \in V$ ?
- **(expressivity)** For a certain class of functions  $\mathcal{K} \subset V$ , determine how fast  $e_n(u) \rightarrow 0$ , or determine the complexity

$$n = n(\varepsilon, \mathcal{K}) \quad \text{s.t.} \quad e_n(u) \leq \varepsilon.$$

Typically, we search for

$$e_n(u) \leq C\gamma(n)^{-1}$$

where  $C \geq 1$ ,  $\gamma$  is a strictly increasing growth function, and

$$n(\varepsilon, u) \geq \gamma^{-1}(\varepsilon/C).$$

- (approximation classes) Characterize the class of functions for which a certain convergence type is achieved, e.g.,

$$\mathcal{A}^\gamma = \{u \in V : \sup_{n \geq 1} \gamma(n) e_n(u) < +\infty\}$$

for some growth function  $\gamma$ .

- (algorithm) Construct an approximation  $u_n \in V_n$  such that

$$\|u - u_n\| \leq C e_n(u) = C \inf_{v \in V_n} \|u - v\|$$

with  $C$  independent of  $n$ .

Algorithms depend on the available information, e.g., given by observations such as point evaluations, or equations satisfied by the functions.

Suppose now that we want to approximate all functions  $u$  from a **compact subset**  $\mathcal{K} \subset V$  (model class).

The quality of an encoding procedure with  $n$  parameters can be measured as:

- In the worst case sense:

$$\mathcal{E}^{\text{wc}}(\mathcal{K}; (E, D)) := \max_{v \in \mathcal{K}} \|v - D(E(v))\|$$

- On average:

$$\mathcal{E}^{\text{av}}(\mathcal{K}; (E, D)) := \int_{\mathcal{K}} \|v - D(E(v))\| d\rho(v)$$

and we can thus define a notion of  $n$ -width

$$\inf_{\substack{(E, D) \\ E: V \rightarrow \mathbb{R}^n \\ D: \mathbb{R}^n \rightarrow V}} \mathcal{E}^{\star}(\mathcal{K}; (E, D)), \quad \star = \{\text{wc}, \text{av}\}$$

by optimizing the choice of  $(E, D)$  under specific restrictions.

$$\inf_{(E,D)} \max_{v \in \mathcal{K}} \|v - D(E(v))\|.$$

We distinguish:

- **Approximation numbers**  $a_n(\mathcal{K})$ : Both  $E$ ,  $D$  are linear:

$$a_n(\mathcal{K}) := \inf_{\substack{L \text{ linear} \\ \text{rank}(L)=n}} \max_{v \in \mathcal{K}} \|v - L(v)\|,$$

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- **Kolmogorov  $n$ -width**  $d_n(\mathcal{K})$ : Only  $D$  is linear

$$d_n(\mathcal{K}) := \inf_{\dim(V_n)=n} \text{dist}(\mathcal{K}, V_n) = \inf_{\dim(V_n)=n} \sup_{u \in \mathcal{K}} \inf_{v \in V_n} \|u - v\|_V$$

We have

$$d_n(\mathcal{K}) \leq a_n(\mathcal{K}),$$

and equality holds in Hilbert spaces.

$d_n(\mathcal{K})$  measures how well the set  $\mathcal{K}$  can be approximated (uniformly) by an  $n$ -dimensional space.

Useful in forward MOR.

$$\inf_{(E,D)} \max_{v \in \mathcal{K}} \|v - D(E(v))\|.$$

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- **Kolmogorov  $n$ -width**  $d_n(\mathcal{K})$ : Only  $D$  is linear
- **Sensing numbers**  $s_n(\mathcal{K})$ : Only  $E$  is linear:

$$s_n(\mathcal{K}) := \inf_{D, \lambda_1, \dots, \lambda_n} \max_{u \in \mathcal{K}} \|u - D(\lambda_1(u), \dots, \lambda_n(u))\|$$

where the inf runs over all  $D$  maps and  $\lambda_j \in V'$ .  
Useful in inverse problems.

$$\inf_{(E,D)} \max_{v \in \mathcal{K}} \|v - D(E(v))\|.$$

We distinguish:

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- **Kolmogorov  $n$ -width**  $d_n(\mathcal{K})$ : Only  $D$  is linear
- **Sensing numbers**  $s_n(\mathcal{K})$ : Only  $E$  is linear:
- **Manifold width**  $\delta_n(\mathcal{K})$ : Both  $E$ ,  $D$  are nonlinear.

$$\inf_{(E,D)} \max_{v \in \mathcal{K}} \|v - D(E(v))\|.$$

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- **Sensing numbers**  $s_n(\mathcal{K})$ : Only  $E$  is linear:
- **Manifold width**  $\delta_n(\mathcal{K})$ : Both  $E$ ,  $D$  are nonlinear.
- **Stable manifold width**  $\delta_n^{\text{cont},\gamma}(\mathcal{K})$ : for robustness against noise perturbations,

$$\delta_n^{\text{cont},\gamma}(\mathcal{K}) := \inf_{(E,D)} \sup_{u \in \mathcal{K}} \|u - D(E(u))\|,$$

where  $E$ ,  $D$  are searched among Lipschitz cont. mappings,

$$\|E(u) - E(v)\|_{\mathbb{R}^n} \leq \gamma \|u - v\|_V, \quad \|D(c) - D(q)\|_V \leq \gamma \|c - q\|_{\mathbb{R}^n}.$$

This concept is studied in [DHM89, CDPW21].

$$\inf_{(E,D)} \max_{v \in \mathcal{K}} \|v - D(E(v))\|.$$

We distinguish:

- **Approximation numbers**  $a_n(\mathcal{K})$ : Both  $E$ ,  $D$  are linear:
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- **Stable manifold width**  $\delta_n^{\text{cont},\gamma}(\mathcal{K})$ : for robustness against noise perturbations,
- We have:

$$a_n(\mathcal{K}) \geq \{d_n(\mathcal{K}), s_n(\mathcal{K})\} \geq \delta_n(\mathcal{K}),$$

$$a_n(\mathcal{K}) \geq \delta_n^{\text{cont},\gamma}(\mathcal{K}) \geq \delta_n(\mathcal{K})$$

The **Kolmogorov  $n$ -width** of  $\mathcal{K}$  is defined as

$$d_n(\mathcal{K}) := \inf_{\dim(V_n)=n} \text{dist}(\mathcal{K}, V_n) = \inf_{\dim(V_n)=n} \sup_{u \in \mathcal{K}} \inf_{v \in V_n} \|u - v\|_V$$

where the infimum runs over all linear subspaces  $V_n$  of dimension  $n$ .

If  $\mathcal{K}$  is equipped with a probability measure  $\pi \in \mathcal{P}(\mathcal{K})$ , we can define a **weighted Kolmogorov  $n$ -width**,

$$d_n^{(p, \pi)} := \inf_{\dim(V_n)=n} \left( \int_{\mathcal{K}} \inf_{v \in V_n} \|u - v\|_V^p d\pi(u) \right)^{1/p}$$

If  $V$  is a Hilbert space,  $p = 2$  and  $\pi$  the push-forward measure of a random variable  $U \in L^2(\Omega, V)$ , this is equivalent to

$$\inf_{\dim(V_n)=n} \int_{\mathcal{K}} \|u(\omega, \cdot) - P_{V_n} u(\omega, \cdot)\|_V^2 d\omega$$

and an optimal space  $V_n$  is given by **Singular Value Decomposition**.

For  $V = L^p(\Omega)$ ,  $\Omega = [0, 1]^d$ ,  $1 \leq p \leq \infty$ , and  $\mathcal{K}$  the unit ball of  $W^{k,p}(\Omega)$ :

$$d_n(\mathcal{K}) \sim n^{-k/d}$$

and optimal performance is obtained by **fixed-knot splines** (with degree adapted to the regularity).

We observe:

- **The curse of dimensionality:** Rate degrades as  $d$  increases.
- **The blessing of smoothness:** Improvement of the rate of approximation when  $k$  increases.
- Few results beyond the classical smoothness classes. However, some crucial results exist for  $\mathcal{K}$  generated by parametric PDEs: we will discuss them in the MOR part.

For  $V = L^p(\Omega)$ ,  $\Omega = [0, 1]^d$ ,  $1 \leq p \leq \infty$ , and  $\mathcal{K}$  the unit ball of  $W^{k,p}(\Omega)$  or Besov spaces  $B_p^k(L^\tau)$  which compactly embed in  $L^p$ , it holds

$$\delta_n^{\text{cont},\gamma}(\mathcal{K}) \sim n^{-k/d}$$

and optimal performance is obtained by, e.g., **free-knot splines** or best  $n$ -term approximation with a dictionary of tensor products of dilated splines. [DHM89]

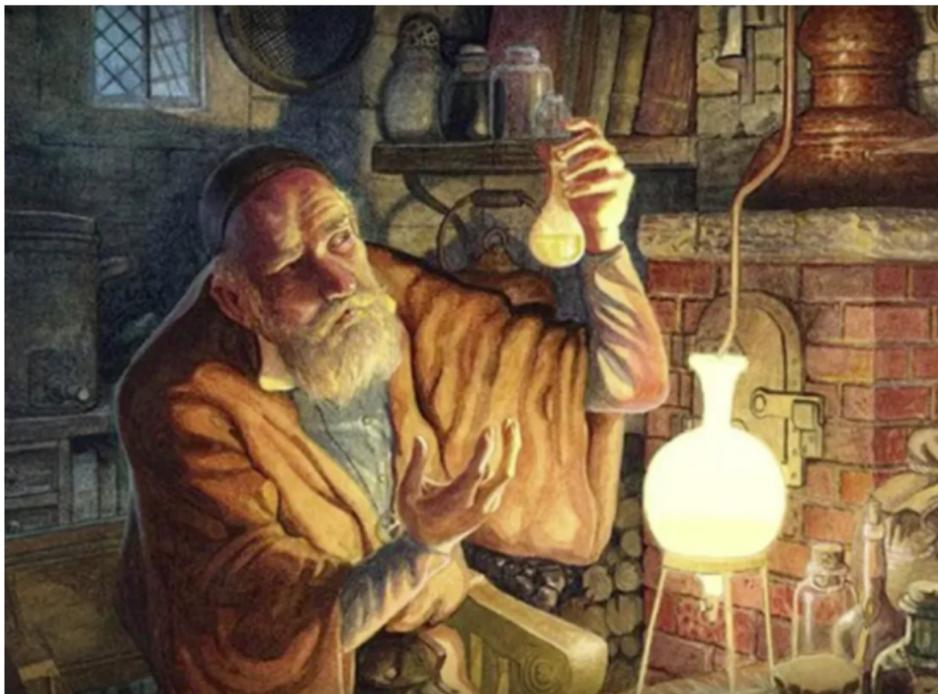
We observe:

- We cover a **larger class of sets than with linear methods**.
- For approximation with **continuous parameters**, the **curse** of dimension is **unavoidable**. What happens for discontinuous parameters?
- Extra regularity does not help: curse of dimension even for  $\mathcal{K} \subset \mathcal{C}^\infty(\Omega)$ .
- These rates do not explain behavior of neural networks.  $\Rightarrow$  Need to consider different approximation classes.

**Part 1.2**  
**Elements of Approximation Theory**  
**The class  $V_n$  of Neural Networks**

## Let us avoid alchemy

To avoid that Machine Learning and DNN become the alchemy of our century, Ali Rahimi asked in 2017 for more rigor, and more theory in his Test-of-Time award's speech. There is still much to do.

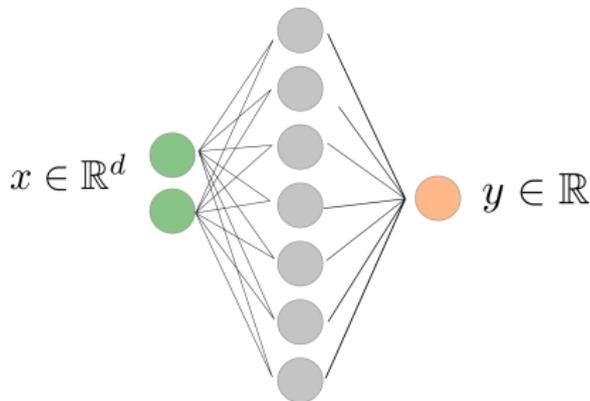


A shallow neural network (with one hidden layer of width  $m$ ) is a function

$$f : \mathbb{R}^d \rightarrow \mathbb{R}$$

$$x \mapsto f(x) := \mathbf{a}^T \sigma(\mathbf{A}x + \mathbf{b}) = \sum_{i=1}^m a_i \sigma \left( \sum_{j=1}^d A_{ij} x_j + b_i \right)$$

where  $\mathbf{a} \in \mathbb{R}^m$ ,  $\mathbf{A} \in \mathbb{R}^{m \times d}$ , and  $\sigma$  is a given nonlinear function (activation function).



**Remark that we can view NN as a nonlinear decoder:**

$$D : \mathbb{R}^n \rightarrow V = \mathbb{F}(\mathbb{R}^d, \mathbb{R})$$

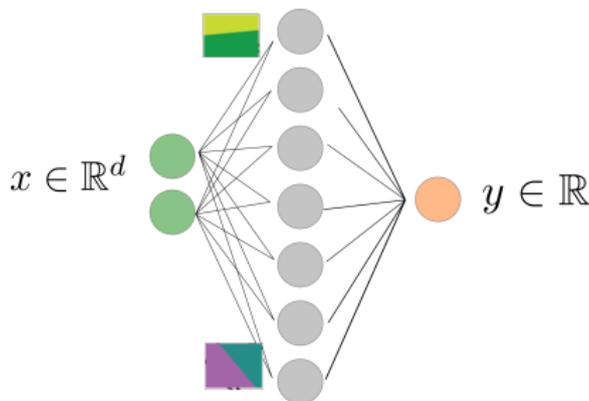
$$c = \{a, A, b\} \mapsto D(c) = f$$

Classical piecewise polynomial activation functions:

- ReLU function  $\sigma(t) = \max\{0, t\}$
- RePU( $p$ ) function  $\sigma(t) = \max\{0, t\}^p$

ReLU and RePU networks produce **free-knot splines**: they are a piecewise polynomial approximation on a free partition of  $\mathbb{R}^d$  determined by  $m$  hyperplanes:

$$H_i = \{x \in \mathbb{R}^d : w_i^T x + b_i = 0\}, \quad w_i = (A_{ij})_{j=1}^d \in \mathbb{R}^d$$



**Universal approximation property:**

The set

$$V_n := \text{span}\{x \in \mathbb{R}^d \mapsto \sigma(w^T x + b) : w \in \mathbb{R}^d, b \in \mathbb{R}\}$$

is dense in  $\mathcal{C}([0, 1]^d)$  if and only if  $\sigma$  is not a polynomial.

Some historical papers on this topic: Cybenko [Cyb89], Hornik [Hor91], Pinkus et al. [LLPS93].

With the universal approximation property, we have addressed the question:

“Can I approximate any continuous function by a neural network?”

And the theorem's answer is

YES provided that the activation functions are not polynomials.

But how much **complexity** (how many terms) do we need to approximate a function to a given **accuracy  $\epsilon$** ? Can the complexity be decreased by leveraging **depth**?

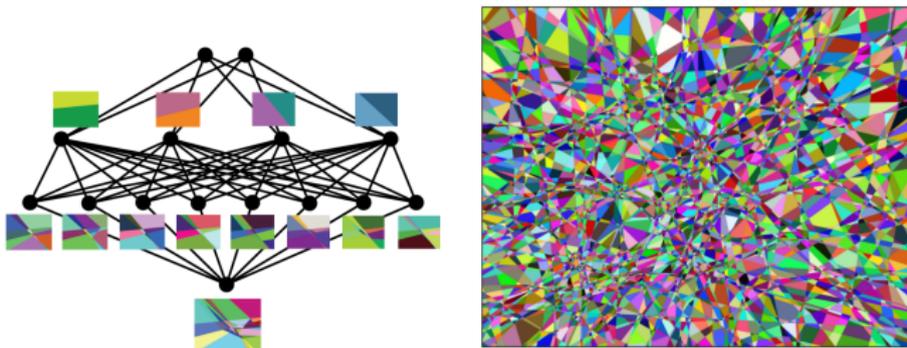
$$f : \mathbb{R}^d \rightarrow \mathbb{R}$$

$$x \mapsto f(x) := T_L \circ \sigma \circ T_{L-1} \circ \sigma \circ \cdots \circ T_1 \circ \sigma \circ T_0(x)$$

with  $T_\ell : \mathbb{R}^{m_\ell} \rightarrow \mathbb{R}^{m_{\ell+1}}$  an affine map

$$T_\ell(x) = A_\ell x + b_\ell, \quad 0 \leq \ell \leq L$$

and  $(m_1, \dots, m_L) \in \mathbb{N}^L$  with  $m_0 = d$ ,  $m_{L+1} = 1$  (or  $m_{L+1} = \vec{d}$ ).



**Figure:** Evolution of linear regions in a DNN with a 2d input (from [HR19])

For a ReLU or REPU( $p$ ) activation function  $\sigma$ , the number of piecewise domains grows exponentially with the depth  $L$ . (free-knot spline)

Frensen, Sasao and Butler prove the following theorem [FSB10]:

Let  $f \in \mathcal{C}^3([a, b])$  and set

$$\kappa := \frac{1}{4} \int_a^b \sqrt{|f''(x)|} dx$$

Let  $\text{CPA}_\varepsilon(f)$  be

$$\text{CPA}_\varepsilon(f) := \{g : [a, b] \rightarrow \mathbb{R} \text{ cont. and piecewise affine s.t. } \|f - g\|_\infty \leq \varepsilon\}$$

The smallest number of segments for a  $g \in \text{CPA}_\varepsilon(f)$  scales as

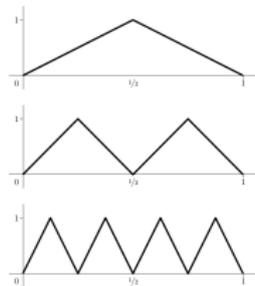
$$s(\varepsilon) \sim \frac{\kappa}{\sqrt{\varepsilon}} \quad \text{as } \varepsilon \rightarrow 0.$$

Complexity of a NN to create that many oscillations?

**Composition creates exponentially many oscillations, addition only linearly many.**

Consider the **sawtooth function**

$$f(x) = \begin{cases} 2x & \text{if } 0 \leq x \leq 1/2 \\ 2 - 2x & \text{if } 1/2 \leq x \leq 1 \end{cases}$$
$$= 2\text{ReLU}(x) - 4\text{ReLU}(x - 1/2)$$



The  $m$ -fold composition  $f_m = f \circ \dots \circ f$  is a function in  $[0, 1]$  with  $2^m - 1$  oscillations.

A function with  $m$  scaled and translated copies has only  $m$  oscillations.

Therefore

$$s(\varepsilon) \sim \frac{\kappa}{\sqrt{\varepsilon}} \quad \Rightarrow \quad m \sim \begin{cases} \ln(\kappa\varepsilon^{-1/2}) \\ \kappa\varepsilon^{-1/2} \end{cases} \quad \begin{array}{l} \text{folds} \\ \text{shallow (translated copies)} \end{array}$$

Let  $\Phi_{L,m}$  be the class of neural networks with depth  $L$  and widths  $m = (m_1, \dots, m_L)$ .

We define

$$V_n := \{v \in \Phi_{L,m} : L \in \mathcal{L}, m \in \mathcal{M}_L, \text{compl}(v) \leq n\}$$

where  $\text{compl}(v)$  is a complexity measure,  $\mathcal{L} \subset \mathbb{N}$  is the set of possible depths and  $\mathcal{M}_L \subset \mathbb{N}^L$  the set of possible widths.

Two typical classes of architectures:

- Fixed depth  $L$  and free width:

$$\mathcal{L} = \{L\}, \quad \mathcal{M}_L = \{(W, \dots, W) : W \in \mathbb{N}\}$$

- Free depth and fixed width  $W$ :

$$\mathcal{L} = \mathbb{N}, \quad \mathcal{M}_L = \{(W, \dots, W)\}$$

## Complexity compl( $v$ )

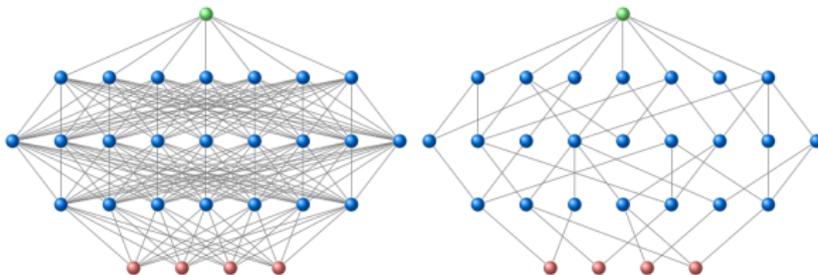
For a function  $v$  in the class  $\Phi_{L,m}$  of neural networks with depth  $L$  and widths  $m = (m_1, \dots, m_L)$ , different measures of complexity:

- number of parameters (fully connected networks):

$$\text{compl}_F(v) = \sum_{\ell=0}^L m_\ell m_{\ell+1} + m_{\ell+1} \sim W^2 L \text{ for } m_\ell \sim W$$

- number of non-zeros parameters (sparsely connected networks)

$$\text{compl}_S(v) = \sum_{\ell=0}^L \|A_\ell\|_0 + \|b_\ell\|_0$$



Structured sparsity can be imposed (convolutional NN, recurrent NN...) or sparsity pattern can be considered as a free parameter (algorithmic challenge).

Suppose  $V = L^2(\Omega)$  is our ambient space, and suppose we take

$$V_n = \Phi_{L,m}, \quad L \text{ fixed, } m = (W, \dots, W)$$

as our approximation set.

For a given target function  $u \in V$ , the error of best approximation is

$$\begin{aligned} e_n(u) &= \inf_{v \in \Phi_{L,m}} \|u - v\|_{L^2(\Omega)} \\ &= \inf_{(A_0, b_0), \dots, (A_L, b_L)} \int_{\Omega} |u(x) - T_L \circ \sigma T_{L-1} \circ \dots \circ \sigma \circ T_0(x)|^2 dx \end{aligned}$$

quantifies the best we can expect from  $V_n$ .

In practice, we throw  $N$  random points  $x_i \in \Omega$ , and we optimize

$$e_n(u) \approx \min_{(A_0, b_0), \dots, (A_L, b_L)} \frac{1}{N} \sum_{i=1}^N |u(x_i) - T_L \circ \sigma T_{L-1} \circ \dots \circ \sigma \circ T_0(x_i)|^2$$

⇒ Questions on optimization and generalization (not covered here).

Many recent results on the expressivity of deep neural networks:

- Approximation classes of DNN (free depth and fixed width) are larger than those of shallow NN (fixed depth and free width) [DDF<sup>+</sup>22].
- **Emulation:** DNN are as expressive as many classical approximation families (polynomials, free-knot splines...).
- They achieve (near to) optimal performance for functions from classical smoothness classes (isotropic and anisotropic Sobolev, Besov, analytic functions...).

Example: For functions  $u \in \mathcal{K} = W^{k,\infty}((0,1)^d)$ , ReLU networks achieve

$$\delta_n^{\text{cont},\gamma}(\mathcal{K})_{L^\infty} := \inf_{E,D} \sup_{u \in \mathcal{K}} \|u - D(E(u))\|,$$

with continuous parameter selection.

- DNN approximate efficiently functions beyond classical smoothness classes (Takagi functions, discontinuous functions, fractals...).

A few surprises:

- In [LSYZ21], it was proven that for functions in  $\mathcal{K} = W^{k,\infty}((0,1)^d)$ , ReLU networks with free depth can achieve

$$e_n(u)_{L^\infty} \lesssim n^{-p} \quad \text{for arbitrary } p \leq 2k/d.$$

However, we said that

$$\delta_n^{\text{cont},\gamma}(\mathcal{K}) \sim n^{-k/d}.$$

Therefore a rate  $p > k/d$  can only be achieved with **discontinuous parameter selection**. Also, it requires more than  $\mathcal{O}(\log_2(\varepsilon^{-1}))$  dofs to achieve accuracy  $\varepsilon$ .

- **Theory-to-practice gap:** No matter how high the theoretically possible approximation rate may be to approximate a given function with a DNN, one requires in practice an **exponential quantity of samples**. [GV21]
- **Personal interpretation:** We need to study DNN approximation for more specific model classes, and derive more closed forms to overcome the curse of dimension, and truly justify the use of NN from the approximation point of view.

## Linear approximation:

- $V_n$  is linear
- Kolmogorov  $n$ -width  $d_n(\mathcal{K})$ : measures optimal linear approx.
- Parametric PDEs:  $d_n(\mathcal{K})$  decays exponentially fast for elliptic/parabolic problems.

## Nonlinear approximation:

- $V_n$  is nonlinear. Usually generated by E, D.
- Manifold  $n$ -width  $\delta_n(\mathcal{K})$ : measures optimal nonlinear approx.
- $\delta_n^{\text{cont}}(\mathcal{K}) \sim n^{-k/d}$  for classical regularity sets. Curse of dimension is unavoidable.
- Neural Networks: emulation, oscillations, efficient beyond classical smoothness classes but no complete picture yet.

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