UAT: From Shallow to Deep

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Logistics

- LaTeX source of homework posted in Canvas (Thanks to Logan Stapleton!)

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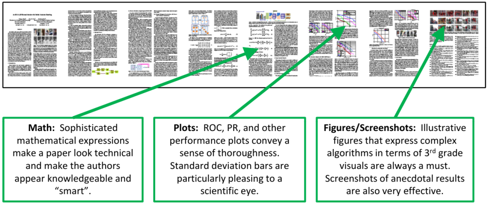

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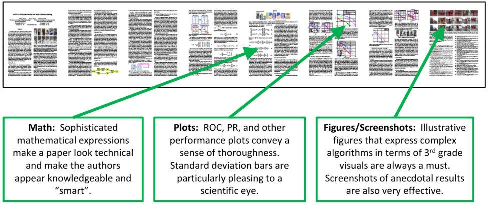


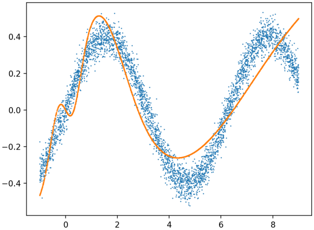
– Matrix Cookbook? Yes and No

Outline

Recap and more thoughts

From shallow to deep NNs

Supervised learning as function approximation



- Underlying true function: f_0
- Training data: $\boldsymbol{y}_i \approx f_0(\boldsymbol{x}_i)$
- Choose a family of functions $\mathcal{H}$, so that $\exists f \in \mathcal{H}$ and

  f and f_0 are close

- **Approximation capacity**: $\mathcal{H}$ matters (e.g., linear? quadratic? sinusoids? etc)
- **Optimization & Generalization**: how to find the best $f \in \mathcal{H}$ matters

We focus on approximation capacity now.

Approximation capacities of NNs

– A single neuron has limited capacity

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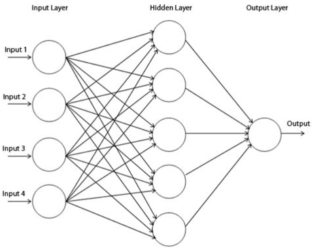
Approximation capacities of NNs

- A single neuron has limited capacity
- Deep NNs with linear activation is no better
- Add in both depth and nonlinearity activation



two-layer network, linear activation at output

universal approximation theorem

> The 2-layer network can approximate **arbitrary** continuous functions **arbitrarily** well, provided that the hidden layer is **sufficiently wide**.

[A] universal approximation theorem (UAT)

Theorem (UAT, [Cybenko, 1989, Hornik, 1991])

Let $\sigma : \mathbb{R} \to \mathbb{R}$ be a nonconstant, bounded, and continuous function. Let I_m denote the m-dimensional unit hypercube $[0,1]^m$. The space of real-valued continuous functions on I_m is denoted by $C(I_m)$. Then, given any $\varepsilon > 0$ and any function $f \in C(I_m)$, there exist an integer N, real constants $v_i, b_i \in \mathbb{R}$ and real vectors $w_i \in \mathbb{R}^m$ for $i = 1, \ldots, N$, such that we may define:

$$F(x) = \sum_{i=1}^{N} v_i \sigma \left(w_i^T x + b_i \right)$$

as an approximate realization of the function f; that is,

$$|F(x) - f(x)| < \varepsilon$$

for all $x \in I_m$.

Thoughts

- Approximate continuous functions with vector outputs, i.e., $I_m \to \mathbb{R}^n$?

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- Map to $[0,1]$, $\{-1,+1\}$, $[0,\infty)$? choose appropriate activation σ at the output

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... universality holds in modified form

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$$F(x) = \boldsymbol{w}^\intercal \sigma(W_2 \sigma(W_1 \boldsymbol{x} + \boldsymbol{b}_1) + \boldsymbol{b}_2) \quad \text{as} \sum_k w_k g_k(\boldsymbol{x})$$

  use w_k's to linearly combine the same function
- **For geeks**: approximate both f and f'?

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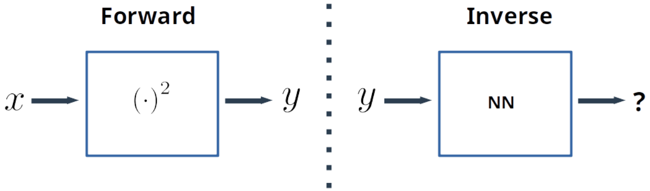

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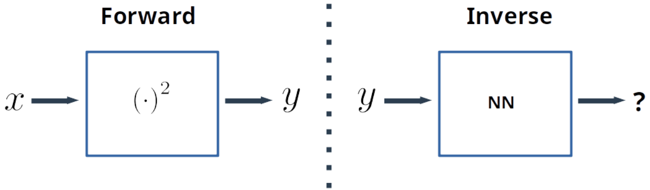

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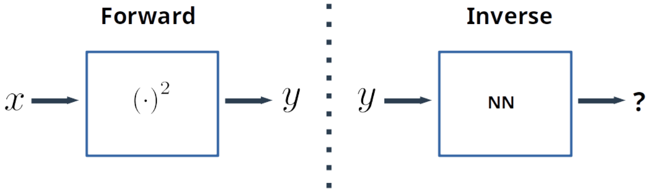

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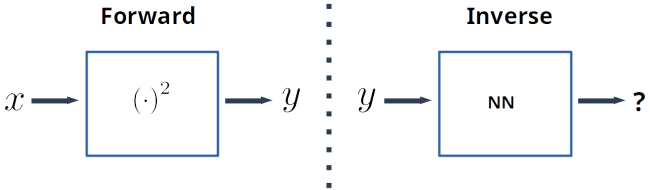

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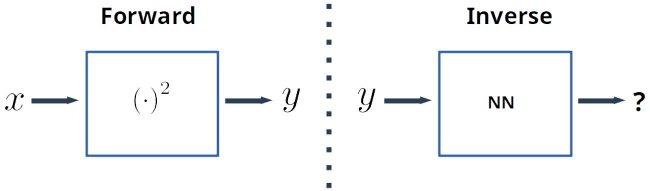

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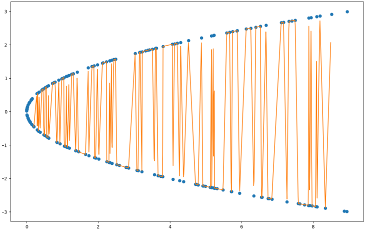
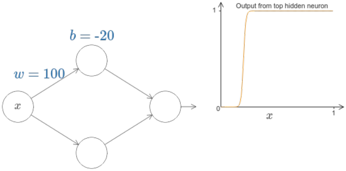
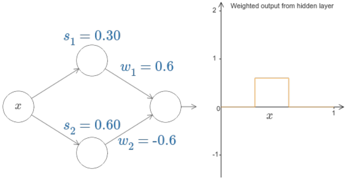
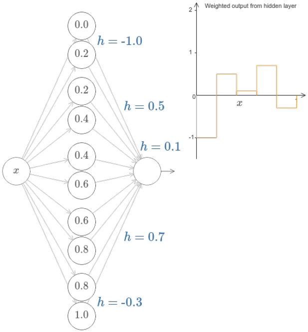
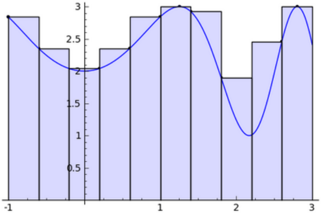


Visual “proof” of UAT

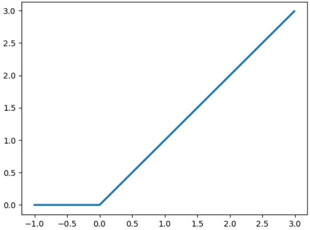








What about ReLU?



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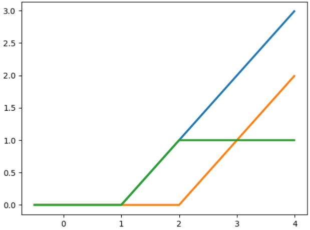

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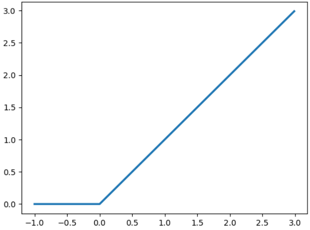

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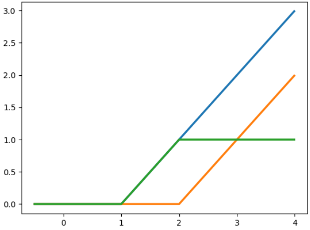

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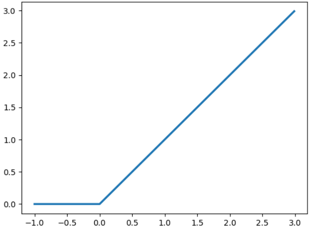

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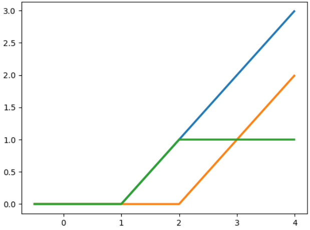

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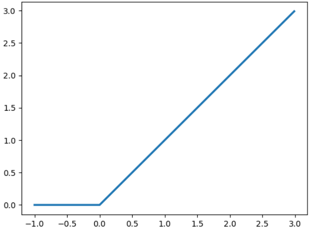

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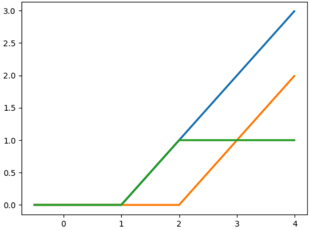

difference of ReLU's

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How general σ can be? ... enough when σ not a polynomial [Leshno et al., 1993]

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Recap and more thoughts

From shallow to deep NNs

What's bad about shallow NNs?

From UAT, "... there exist an interger N, ...", but how large?

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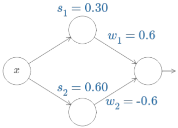
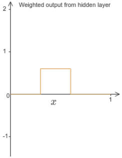
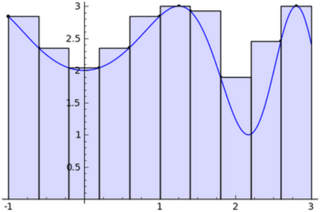
What happens in $1D$?







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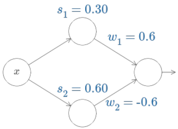

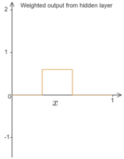

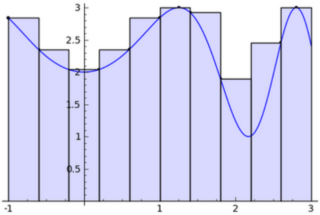

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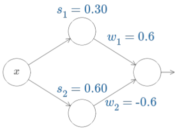

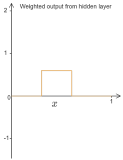

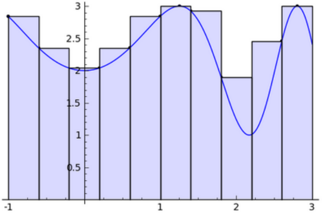

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For ε accuracy, need $\frac{1}{\varepsilon}$ bumps

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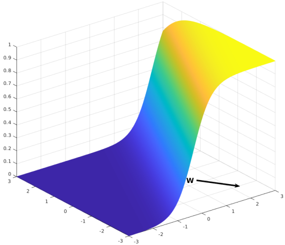
What happens in $2D$? Visual proof in 2D first



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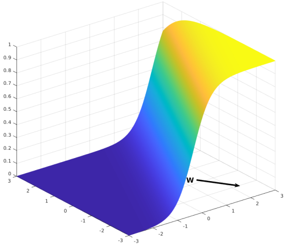
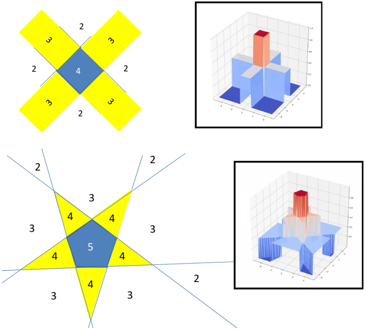


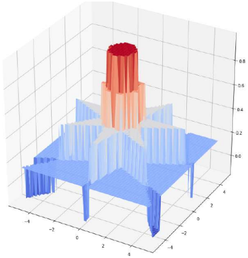
$\sigma(\boldsymbol{w}^\intercal \boldsymbol{x} + \boldsymbol{b})$, σ sigmod approach 2D step function when making $\boldsymbol{w}$ large



Credit: CMU 11-785

Visual proof for 2D functions

Keep increasing the number of step functions that are distributed evenly ...



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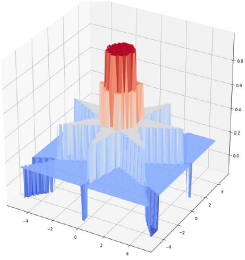

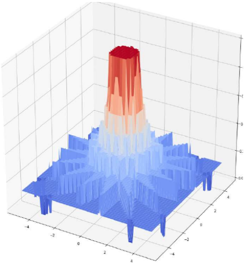

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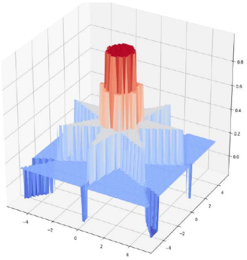

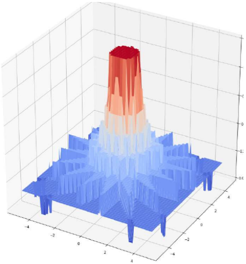

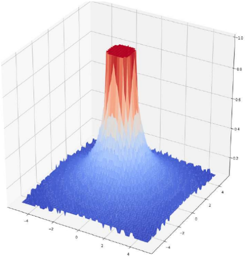

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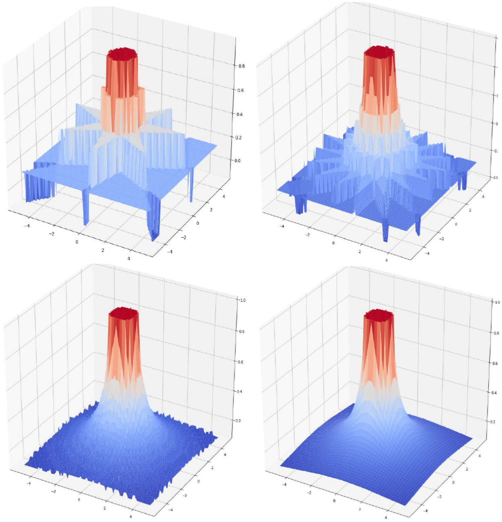

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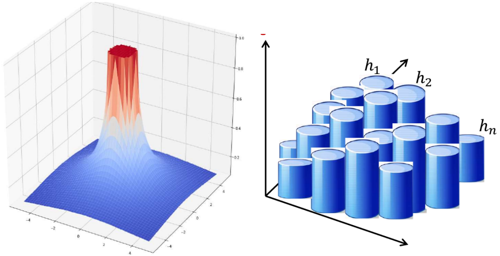

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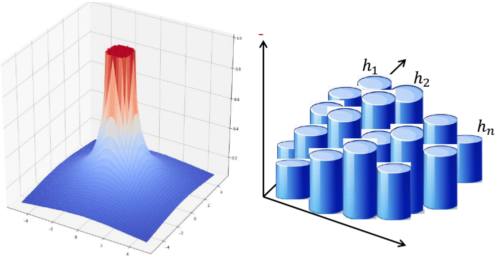

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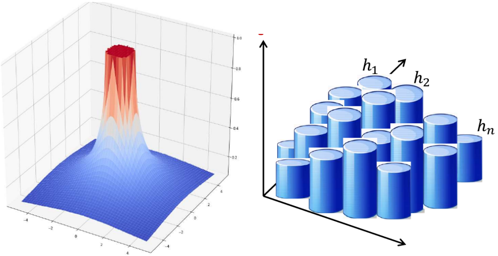

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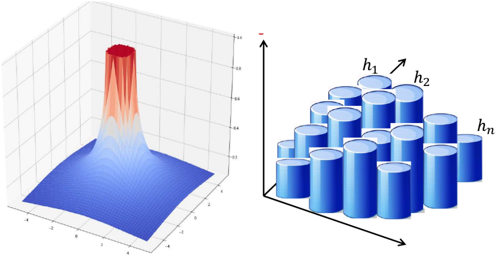
Assume the target f is 1-Lipschitz, i.e., $|f(\boldsymbol{x}) - f(\boldsymbol{y})| \leq \|\boldsymbol{x} - \boldsymbol{y}\|_2, \forall\, \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^2$

For ε accuracy, need $O\left(\varepsilon^{-2}\right)$ bumps.

What's bad about shallow NNs?

From UAT, "... there exist an interger N, ...", but how large?

What happens in $2D$?



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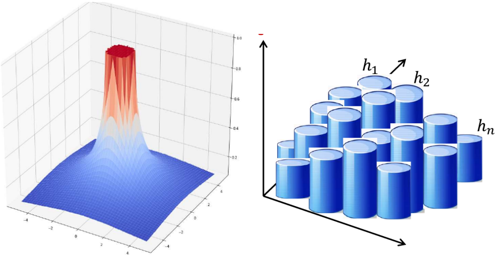

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For ε accuracy, need $O\left(\varepsilon^{-2}\right)$ bumps. What about the n-D case? $O(\varepsilon^{-n})$.

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Learn Boolean functions ($f : \{+1, -1\}^n \mapsto \{+1, -1\}$): DNNs can have #nodes linear in n, whereas 2-layer NN needs exponential nodes (more in HW1)

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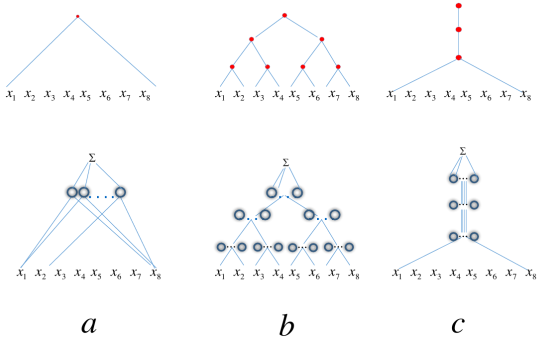

A family: compositional function [Poggio et al., 2017]

Compositional functions

$$f(x_1, \cdots, x_8) = h_3(h_{21}(h_{11}(x_1, x_2), h_{12}(x_3, x_4)), \\ h_{22}(h_{13}(x_5, x_6), h_{14}(x_7, x_8))) \quad (4)$$

W_m^n: class of n-variable functions with partial derivatives up to m-th order, $W_m^{n,2} \subset W_m^n$ is the compositional subclass following binary tree structures

Theorem 1. *Let $\sigma : \mathbb{R} \to \mathbb{R}$ be infinitely differentiable, and not a polynomial. For $f \in W_m^n$ the complexity of shallow networks that provide accuracy at least ϵ is*

$$N = \mathcal{O}(\epsilon^{-n/m}) \text{ and is the best possible.} \quad (5)$$

Theorem 2. *For $f \in W_m^{n,2}$ consider a deep network with the same compositonal architecture and with an activation function $\sigma : \mathbb{R} \to \mathbb{R}$ which is infinitely differentiable, and not a polynomial. The complexity of the network to provide approximation with accuracy at least ϵ is*

$$N = \mathcal{O}((n-1)\epsilon^{-2/m}). \quad (6)$$

from [Poggio et al., 2017] ; see Sec 4.2 of [Poggio et al., 2017] for lower bound

Nonsmooth activation

A terse version of UAT

Proposition 2. *Let* $\sigma =: \mathbb{R} \to \mathbb{R}$ *be in* $\mathcal{C}^0$*, and not a polynomial. Then shallow networks are dense in* $\mathcal{C}^0$*.*

Nonsmooth activation

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Shallow vs. deep

Theorem 4. *Let f be a L-Lipshitz continuous function of n variables. Then, the complexity of a network which is a linear combination of ReLU providing an approximation with accuracy at least ϵ is*

$$N_s = \mathcal{O}\left(\left(\frac{\epsilon}{L}\right)^{-n}\right),$$

wheres that of a deep compositional architecture is

$$N_d = \mathcal{O}\left(\left(n-1)(\frac{\epsilon}{L}\right)^{-2}\right).$$

from [Poggio et al., 2017]

Width-bounded DNNs

Narrower than $n + 4$ is fine

Theorem 1 (Universal Approximation Theorem for Width-Bounded ReLU Networks). *For any Lebesgue-integrable function $f : \mathbb{R}^n \to \mathbb{R}$ and any $\epsilon > 0$, there exists a fully-connected ReLU network $\mathscr{A}$ with width $d_m \leq n + 4$, such that the function $F_{\mathscr{A}}$ represented by this network satisfies*

$$\int_{\mathbb{R}^n} |f(x) - F_{\mathscr{A}}(x)| \mathrm{d}x < \epsilon. \quad (3)$$

But no narrower than $n - 1$

Theorem 3. *For any continuous function $f : [-1, 1]^n \to \mathbb{R}$ which is not constant along any direction, there exists a universal $\epsilon^* > 0$ such that for any function F_A represented by a fully-connected ReLU network with width $d_m \leq n - 1$, the L^1 distance between f and F_A is at least ϵ^*:*

$$\int_{[-1,1]^n} |f(x) - F_A(x)| \mathrm{d}x \geq \epsilon^*. \quad (5)$$

from [Lu et al., 2017]; see also [Kidger and Lyons, 2019]

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Deep vs. shallow still active area of research

Number one principle of DL

Fundamental theorem of DNNs

Universal approximation theorems

Number one principle of DL

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Universal approximation theorems

Fundamental slogan of DL

Where there is a mapping, there is a NN... and fit it!

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