Fundamental Belief: Universal Approximation Theorems

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Logistics

– HW 0 posted (due: midnight Sep 30)

HOMEWORK SET 0

CSCI 5980/8980 Think Deep Learning (Fall 2020)

Due 11:59 pm, Sep 30 2020

Instruction Please typeset your homework in LaTeX and submit it as a single PDF file in Canvas. No late submission will be accepted. For each problem, your should acknowledge your collaborators if any. For problems containing multiple subproblems, there are often close logic connections between the subproblems. So always remember to build on previous ones, rather than work from scratch.

Notation We will use small letters (e.g., u) for scalars, small boldface letters (e.g., $\boldsymbol{a}$) for vectors, and capital boldface letters (e.g., $\boldsymbol{A}$) for matrices. $\mathbb{R}$ is the set of real numbers. $\mathbb{R}^n$ is the space of n-dimensional real vectors, and similarly $\mathbb{R}^{m \times n}$ is the space of $m \times n$ real matrices. The dotted equal sign $\doteq$ means defining.

Problem 1 (Chain rules, gradient and Hessian) Recall from calculus that for a multivariate function $f(\boldsymbol{x})$ mapping from $\mathbb{R}^n$ to $\mathbb{R}$, i.e., $f : \mathbb{R}^n \mapsto \mathbb{R}$, the i-th partial derivative of f is defined as $\frac{\partial f}{\partial x_i}$, i.e., the univariate derivative with respect to the i-th variable while holding the other variables constant. This generalizes naturally to the matrix case, where we consider $f(\boldsymbol{X})$ with $\boldsymbol{X} \in \mathbb{R}^{m \times n}$.

– CSCI8980 lecture scribing (2 scribers per session, 2 reviewers per session)

– Review of Scipy, Numpy, MSI resource, Colab + Project ideas (Sep 28 or Oct 05, TBD)

Typesetting and matrix calculus

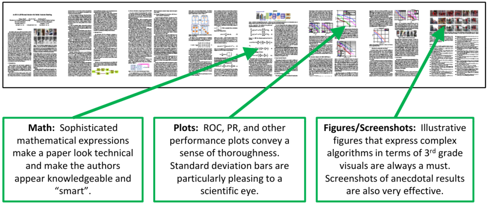
- $\LaTeX$ source of homework also posted in Canvas

  Mind $\LaTeX$! Mind your math!

  * Ten Signs a Claimed Mathematical Breakthrough is Wrong

    > Inspired by Sean Carroll's closely-related Alternative-Science Respectability Checklist, without further ado I now offer the *Ten Signs a Claimed Mathematical Breakthrough is Wrong*.
    >
    > **1. The authors don't use TeX.** This simple test (suggested by Dave Bacon) already catches at least 60% of wrong mathematical breakthroughs. David Deutsch and Lov Grover are among the only known false positives.

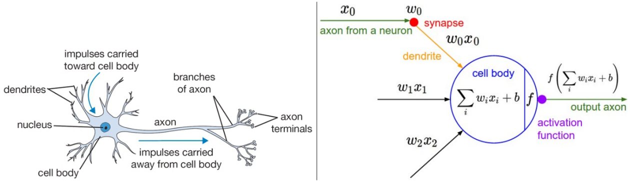
  * Paper Gestalt $(50\%/18\%$, 2009) $\Longrightarrow$ Deep Paper Gestalt $(50\%/0.4\%$, 2018)



- Matrix Cookbook? Yes and No

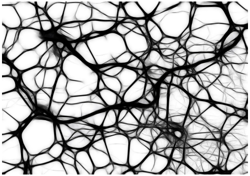
  http://www2.imm.dtu.dk/pubdb/pubs/3274-full.html

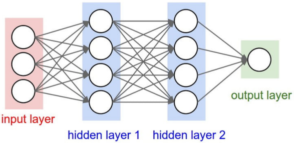
Outline



A cartoon drawing of a biological neuron (left) and its mathematical model (right).

biological neuron vs. **artificial neuron**



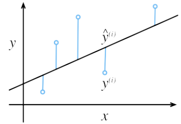


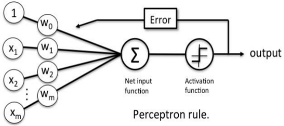
biological NN vs. **artificial NN**

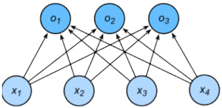
Artificial NN: (over)-simplification on **neuron** & **connection** levels

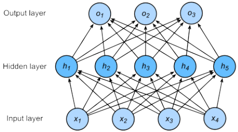
Recap II

Zoo of NN models in ML







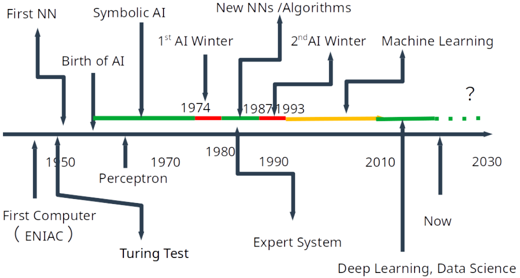


- Linear regression
- Perception and Logistic regression
- Softmax regression
- Multilayer perceptron (feedforward NNs)

Also:

- Support vector machines (SVM)
- PCA (autoencoder)
- Matrix factorization

Recap III



Brief history of NNs:

- 1943: first NNs invented (McCulloch and Pitts)
- 1958 –1969: perceptron (Rosenblatt)
- 1969: *Perceptrons* (Minsky and Papert)—end of perceptron
- 1980's–1990's: Neocognitron, CNN, back-prop, SGD—we use today
- 1990's–2010's: SVMs, Adaboosting, decision trees and random forests
- 2010's–now: DNNs and deep learning

Outline

Supervised learning

General view:

- Gather training data $(\boldsymbol{x}_1, \boldsymbol{y}_1), \dots, (\boldsymbol{x}_n, \boldsymbol{y}_n)$
- Choose a family of functions, e.g., $\mathcal{H}$, so that there is $f \in \mathcal{H}$ to ensure $\boldsymbol{y}_i \approx f(\boldsymbol{x}_i)$ for all i
- Set up a loss function ℓ
- Find an $f \in \mathcal{H}$ to minimize the average loss

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(\boldsymbol{y}_i, f(\boldsymbol{x}_i))$$

NN view:

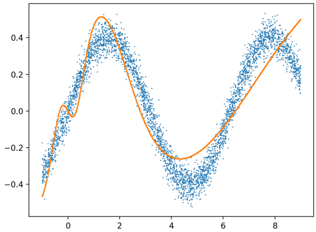
- Gather training data $(\boldsymbol{x}_1, \boldsymbol{y}_1), \dots, (\boldsymbol{x}_n, \boldsymbol{y}_n)$
- Choose a NN with k neurons, so that there is a group of weights, e.g., $(\boldsymbol{w}_1, \dots, \boldsymbol{w}_k, b_1, \dots, b_k)$, to ensure $\boldsymbol{y}_i \approx \{\mathsf{NN}(\boldsymbol{w}_1, \dots, \boldsymbol{w}_k, b_1, \dots, b_k)\}(\boldsymbol{x}_i) \quad \forall i$
- Set up a loss function ℓ
- Find weights $(\boldsymbol{w}_1, \dots, \boldsymbol{w}_k, b_1, \dots, b_k)$ to minimize the average loss

$$\min_{\boldsymbol{w}'s, b's} \frac{1}{n} \sum_{i=1}^{n} \ell\left[\boldsymbol{y}_i, \{\mathsf{NN}(\boldsymbol{w}_1, \dots, \boldsymbol{w}_k, b_1, \dots, b_k)\}(\boldsymbol{x}_i)\right]$$

Why should we trust NNs?

Function approximation

More accurate description of supervised learning



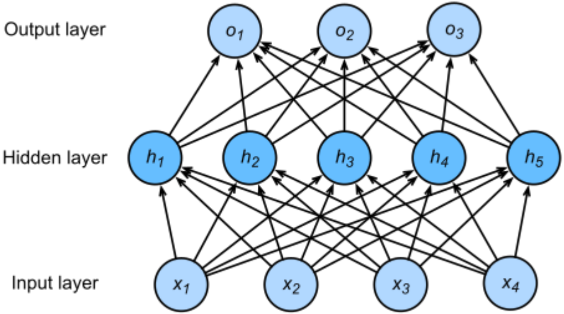
- Underlying true function: f_0
- Training data: $\boldsymbol{y}_i \approx f_0(\boldsymbol{x}_i)$
- Choose a family of functions $\mathcal{H}$, so that $\exists f \in \mathcal{H}$ and

  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.

A word on notation

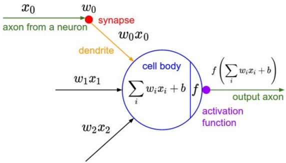


- k-layer NNs: with k layers of weights (along the deepest path)
- k-hidden-layer NNs: with k hidden layers of nodes (i.e., $(k+1)$-layer NNs)

First trial

Think of single-output (i.e., $\mathbb{R}^n \mapsto \mathbb{R}$) problems first

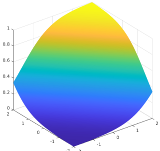
A single neuron

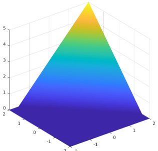


($f \to \sigma$: again, activation always as σ)

$$\mathcal{H} : \{\boldsymbol{x} \mapsto \sigma\left(\boldsymbol{w}^\intercal \boldsymbol{x} + b\right)\}$$

- σ identity or linear: linear functions
- σ sign function $\mathrm{sign}\left(\boldsymbol{w}^\intercal \boldsymbol{x} + b\right)$ (perceptron): $0/1$ function with hyperplane threshold
- $\sigma = \frac{1}{1+e^{-z}}$: $\left\{\boldsymbol{x} \mapsto \frac{1}{1+e^{-(\boldsymbol{w}^\intercal \boldsymbol{x}+b)}}\right\}$
- $\sigma = \max(0, z)$ (ReLU): $\{\boldsymbol{x} \mapsto \max(0, \boldsymbol{w}^\intercal \boldsymbol{x} + b)\}$

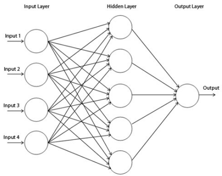


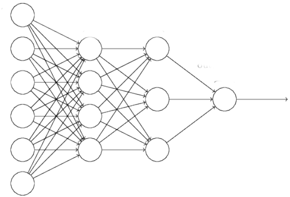


Second trial

Think of single-output (i.e., $\mathbb{R}^n \mapsto \mathbb{R}$) problems first

Add depth!





...

But make all hidden-nodes activations identity or linear

$$\sigma\left(\boldsymbol{w}_L^\intercal\left(\boldsymbol{W}_{L-1}\left(\ldots\left(\boldsymbol{W}_1\boldsymbol{x}+\boldsymbol{b}_1\right)+\ldots\right)\boldsymbol{b}_{L-1}\right)+b_L\right)$$

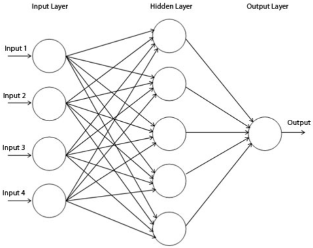
No better than a signle neuron!

Why?

Third trial

Think of single-output (i.e., $\mathbb{R}^n \mapsto \mathbb{R}$) problems first

Add both depth & nonlinearity!



two-layer network, linear activation at output

Surprising news:
universal approximation theorem

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

— so we don't worry about limitation in the capacity

Outline

Why could UAT hold?

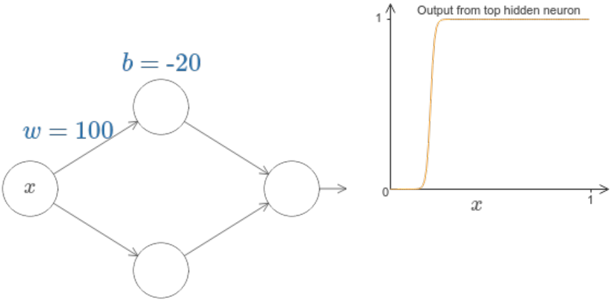
Visual "proof"

(http://neuralnetworksanddeeplearning.com/chap4.html)

Think of $\mathbb{R} \to \mathbb{R}$ functions first, $\sigma = \frac{1}{1+e^{-z}}$

- Step 1: Build "step" functions
- Step 2: Build "bump" functions
- Step 3: Sum up bumps to approximate

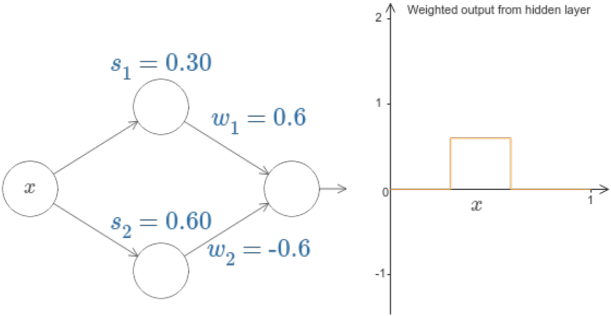
Step 1: build step functions



$$y = \frac{1}{1 + e^{-(wx+b)}} = \frac{1}{1 + e^{-w(x-b/w)}}$$

- Larger w, sharper transition
- Transition around $-b/w$, written as s

Step 2: build bump functions

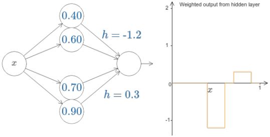


$$0.6 * \text{step}(0.3) - 0.6 * \text{step}\,(0.6)$$

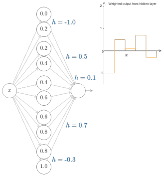
Write h as the bump height

Step 3: sum up bumps to approximate

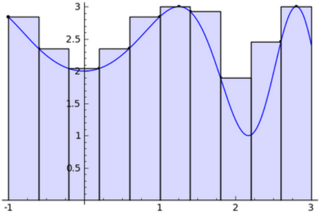
two bumps



five bumps



ultimate idea ... familiar?



Message: all $\mathbb{R} \mapsto \mathbb{R}$ functions can be "well" approximated using 2-layer NN's

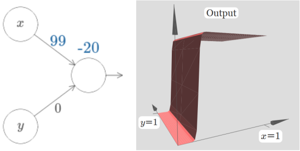
What about high-dimensional?

Similar story

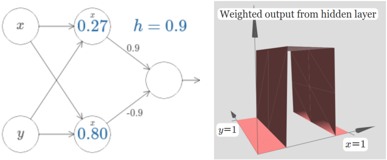
- Step 1: Build "step" functions
- Step 2: Build "bump" functions
- Step 3: Build "tower" functions
- Step 4: Sum up bumps to approximate

http://neuralnetworksanddeeplearning.com/chap4.html

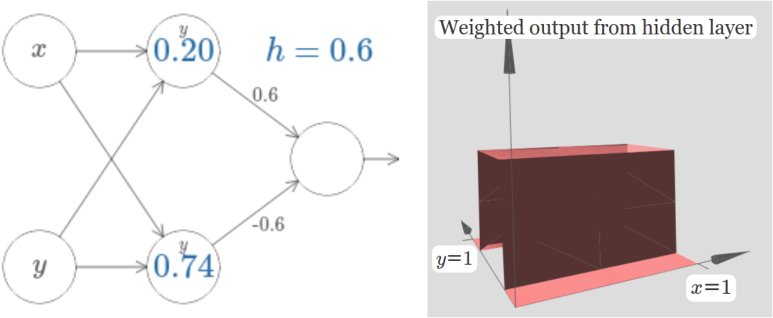
Steps 1 & 2: build step and bump functions



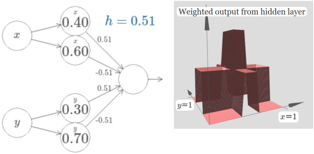
step in x by setting large weight for x



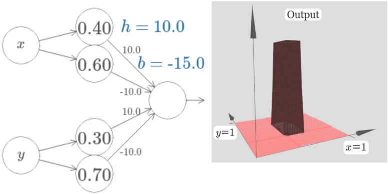
bump in x by diff of two steps in x



Step 3: build tower functions

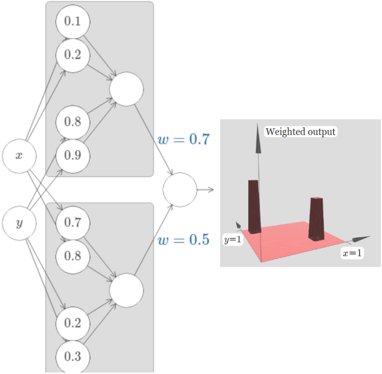


sum up x, y bumps to obtain a stair tower

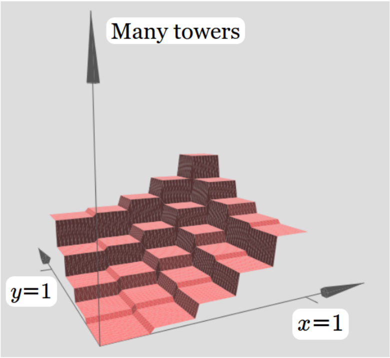


threshold to obtain a sharp tower

Step 4: sum up towers for approximation



sum up two towers



sum up many towers

Message: all $\mathbb{R}^2 \mapsto \mathbb{R}$ functions can be "well" approximated using 3-**layer** NN's Question: Possible using 2-layer NNs only?

General cases?

- What about $\mathbb{R}^n \mapsto \mathbb{R}$ functions?
  The "step $\rightarrow$ (bump) $\rightarrow$ tower $\rightarrow$ tower array" construction carries over
- What about $\mathbb{R}^n \mapsto \mathbb{R}^m$ functions?
  Approximate each $\mathbb{R}^n \mapsto \mathbb{R}$ separately and then glue them together

Message: All $\mathbb{R}^n \mapsto \mathbb{R}^m$ functions can be "well" approximated using 2-layer NN's

Outline

[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:

$$F(\boldsymbol{x}) = \sum_{i=1}^{N} v_i \sigma \left(\boldsymbol{w}_i^T \boldsymbol{x} + b_i \right) = \boldsymbol{v}^\intercal \sigma \left(\boldsymbol{W}^\intercal \boldsymbol{x} + \boldsymbol{b} \right)$$

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

$$|F(\boldsymbol{x}) - f(\boldsymbol{x})| < \varepsilon$$

for all $\boldsymbol{x} \in I_m$.

Rigorous proof?

The proof is very technical ... functional analysis

1. Riesz Representation: Every linear functional on $C^0([0,1]^k)$ is given by
$$f \mapsto \int_{[0,1]^k} f(x) d\mu(x), \qquad \mu \in \mathcal{M}$$
where $\mathcal{M} = \left\{\text{finite signed regular Borel measures on } [0,1]^k\right\}$.

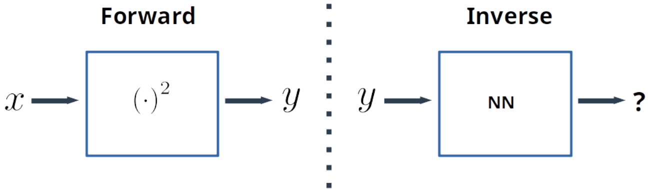
2. **Lemma.** Suppose for each $\mu \in \mathcal{M}$, we have
$$\int_{[0,1]^k} \phi(w \cdot x + b) d\mu(x) = 0 \quad \forall w, b \quad \Rightarrow \quad \mu = 0. \quad (0.1)$$
Then $\mathrm{Nets}_1(\phi)$ is dense in $C^0([0,1]^k)$.

3. **Lemma.** ϕ continuous, sigmoidal $\quad \Rightarrow \quad$ satisfies (0.1).

Thoughts on UAT

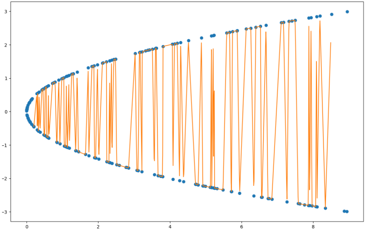
- $\sigma : \mathbb{R} \to \mathbb{R}$ **be a nonconstant, bounded, and continuous**: what about ReLU (leaky ReLU) or sign function (as in perceptron)? We have many UAT **theorem(s)**
- I_m **denote the m-dimensional unit hypercube** $[0, 1]^m$: this can replaced by any compact subset of $\mathbb{R}^m$
- **there exist an integer** N: but how large N needs to be? (later)
- **The space of real-valued continuous functions on** I_m: two examples to ponder on
  - binary classification
  - learn to solve square root

Learn to take square-root



Suppose we lived in a time square-root is not defined ...

- Training data: $\{x_i, x_i^2\}_i$, where $x_i \in \mathbb{R}$
- Forward: if $x \mapsto y$, $-x \mapsto y$ also
- To invert, what to output? What if just throw in the training data?



Thoughts

- Approximate continuous functions with vector outputs, i.e., $I_m \to \mathbb{R}^n$? think of the component functions
- Map to $[0,1]$, $\{-1,+1\}$, $[0,\infty)$? choose appropriate activation σ at the output

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

  ... universality holds in modified form

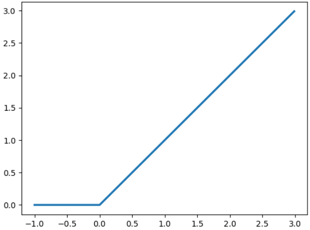
- Get deeper? three-layer NN? change to matrix-vector notation for convenience

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

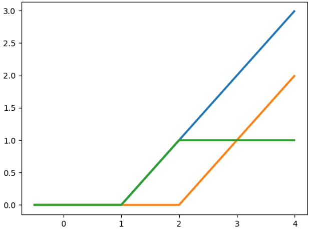
  use w_k's to linearly combine the same function

- **For geeks**: approximate both f and f'? check out [Hornik et al., 1990]

What about ReLU?



ReLU



difference of ReLU's

what happens when the slopes of the ReLU's are changed?

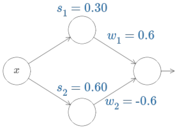
How general σ can be? ... enough when σ not a polynomial [Leshno et al., 1993]

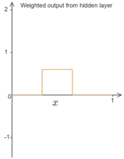
Outline

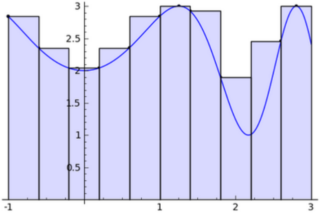
What's bad about shallow NNs?

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

What happens in $1D$?







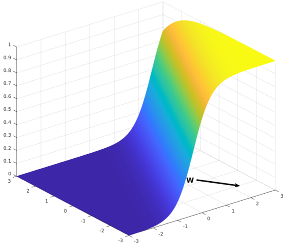
Assume the target f is 1-Lipschitz, i.e., $|f(x) - f(y)| \leq |x - y|, \forall\, x, y \in \mathbb{R}$

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

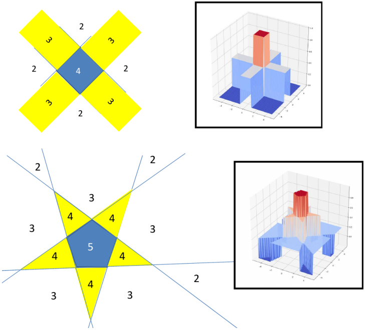
What's bad about shallow NNs?

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

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



$\sigma(\boldsymbol{w}^\intercal \boldsymbol{x} + \boldsymbol{b})$, 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 ...

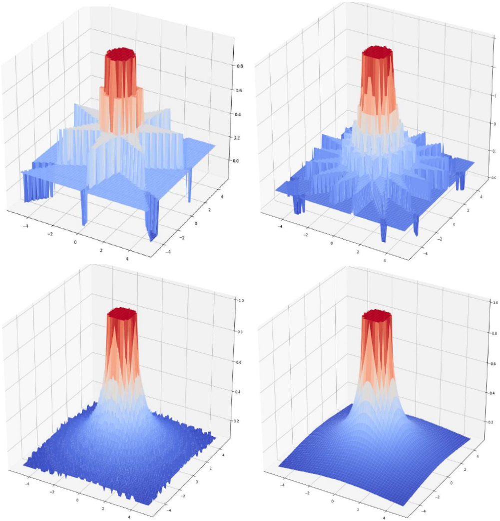


Image Credit: CMU 11-785

What's bad about shallow NNs?

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

What happens in $2D$?

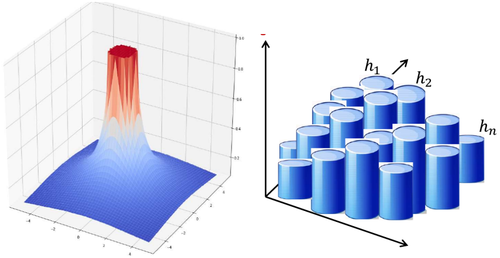


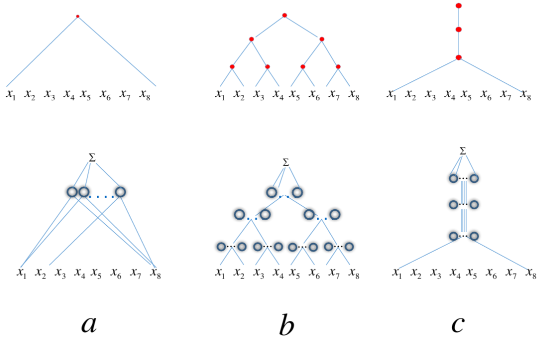
Image Credit: CMU 11-785

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 about the n-D case? $O(\varepsilon^{-n})$.

What's good about deep NNs?

- 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)
- What general functions set deep and shallow NNs apart?



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 $\mathcal{C}^0$.*

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*

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

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^*:*

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

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

Deep vs. shallow still active area of research

Number one principle of DL

Fundamental theorem of DNNs

Universal approximation theorems

Fundamental slogan of DL

Where there is a function, there is a NN...
and go ahead fitting it!

Outline

Suggested reading

- Chap 4, Neural Networks and Deep Learning (online book) http://neuralnetworksanddeeplearning.com/chap4.html
- Why and when can deep-but not shallow-networks avoid the curse of dimensionality: A review. (by Poggio et al) https://arxiv.org/abs/1611.00740
- Expressivity of Deep Neural Networks (by Ingo Gühring, Mones Raslan, Gitta Kutyniok) https://arxiv.org/abs/2007.04759

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References ii

[Poggio et al., 2017] Poggio, T., Mhaskar, H., Rosasco, L., Miranda, B., and Liao, Q. (2017). **Why and when can deep-but not shallow-networks avoid the curse of dimensionality: A review.** *International Journal of Automation and Computing*, 14(5):503–519.