Compare Shallow and Deep Neural Network for Function Approximation

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Reference Paper

Liang, Shiyu and R. Srikant. “Why Deep Neural Networks for Function Approximation?” International Conference on Learning Representations (2017) [1].

Shallow networks need exponentially more neurons than deep networks to approximate a function.

Goal

Focus on bounds on the size of deep network for function approximation to guarantee an ε-approximation.

Given a function f, our goal is to find out whether a deep neural network ˜f of upper bounds on the depth L(ε) and size N(ε) exists such that it solves $\min_{\tilde{f} \in \mathcal{F}(N,L)} \|f - \tilde{f}\| \leq \varepsilon.$

Approximation of univariate functions.

Then extend these results to certain classes of multivariate functions.

Theorem 1 of Univariate Function

Theorem 1. *For function* $f(x) = x^2, x \in [0,1]$*, there exists a multilayer neural network* $\tilde{f}(x)$ *with* $\mathcal{O}\left(\log \frac{1}{\varepsilon}\right)$ *layers,* $\mathcal{O}\left(\log \frac{1}{\varepsilon}\right)$ *binary step units and* $\mathcal{O}\left(\log \frac{1}{\varepsilon}\right)$ *rectifier linear units such that* $|f(x) - \tilde{f}(x)| \leq \varepsilon, \quad \forall x \in [0,1]$.

Theorem of approximating a quadratic function.

Proof

For any x ∈ [0, 1], we first use the multilayer neural network to approximate x by its finite binary expansion $\sum_{i=0}^{n} \frac{x_i}{2^i}$

Next, implement the function $\tilde{f}(x) = f\left(\sum_{i=0}^{n} \frac{x_i}{2^i}\right)$ by a two-layer neural network

Since f(x) = x^2, we can further get: $\tilde{f}(x) = \left(\sum_{i=0}^{n} \frac{x_i}{2^i}\right)^2 = \sum_{i=0}^{n}\left[x_i \cdot \left(\frac{1}{2^i}\sum_{j=0}^{n}\frac{x_j}{2^j}\right)\right] = \sum_{i=0}^{n} \max\left(0, 2(x_i - 1) + \frac{1}{2^i}\sum_{j=0}^{n}\frac{x_j}{2^j}\right).$

The approximate error function can then be considered as:

$$|f(x) - \tilde{f}(x)| = \left| x^2 - \left(\sum_{i=0}^{n} \frac{x_i}{2^i}\right)^2 \right| \leq 2\left| x - \sum_{i=0}^{n} \frac{x_i}{2^i} \right| = 2\left| \sum_{i=n+1}^{\infty} \frac{x_i}{2^i} \right| \leq \frac{1}{2^{n-1}}.$$

In order to achieve ε-approximation error, $n = \left\lceil \log_2 \frac{1}{\varepsilon} \right\rceil + 1$

Since we used O(n + p) layers with O(n) binary step units and O(pn) rectifier linear units in total, the deep neural network has O(log 1/ε) layers, O(log 1/ε) binary step units and O(log 1/ε) rectifier linear units.

Theorem 2 of Univariate Function

Theorem 2. *For polynomials* $f(x) = \sum_{i=0}^{p} a_i x^i$, $x \in [0,1]$ *and* $\sum_{i=1}^{p} |a_i| \leq 1$, *there exists a multilayer neural network* $\tilde{f}(x)$ *with* $\mathcal{O}\left(p + \log \frac{p}{\varepsilon}\right)$ *layers,* $\mathcal{O}\left(\log \frac{p}{\varepsilon}\right)$ *binary step units and* $\mathcal{O}\left(p \log \frac{p}{\varepsilon}\right)$ *rectifier linear units such that* $|f(x) - \tilde{f}(x)| \leq \varepsilon, \forall x \in [0,1]$.

Theorem of the network for approximating general polynomials.

Proof

First use the deep structure to find the n-bit binary expansion $\sum_{i=0}^{n} a_i x^i$ of x.

Then construct a multilayer network to approximate polynomials gi(x) = x^i , i=1,...,p, rewrite it as $g_{m+1}(\sum_{i=0}^{n} \frac{x_i}{2^n})$

$$g_{m+1}\left(\sum_{i=0}^{n}\frac{x_i}{2^i}\right)=\sum_{j=0}^{n}\left[x_j\cdot\frac{1}{2^j}g_m\left(\sum_{i=0}^{n}\frac{x_i}{2^i}\right)\right]=\sum_{j=0}^{n}\max\left[2(x_j-1)+\frac{1}{2^j}g_m\left(\sum_{i=0}^{n}\frac{x_i}{2^i}\right),0\right]$$

The expansion defines iterations between the outputs of neighbor layers.

Proof

Define the output of the multilayer neural network as: $\tilde{f}(x) = \sum_{i=0}^{p} a_i g_i \left(\sum_{j=0}^{n} \frac{x_j}{2^j} \right)$

For this deep network, the approximation error is:

$$|f(x) - \tilde{f}(x)| = \left| \sum_{i=0}^{p} a_i g_i \left(\sum_{j=0}^{n} \frac{x_j}{2^j} \right) - \sum_{i=0}^{p} a_i x^i \right| \leq \sum_{i=0}^{p} \left[|a_i| \cdot \left| g_i \left(\sum_{j=0}^{n} \frac{x_j}{2^j} \right) - x^i \right| \right] \leq \frac{p}{2^{n-1}}$$

Choose n = log (p/ε) + 1.

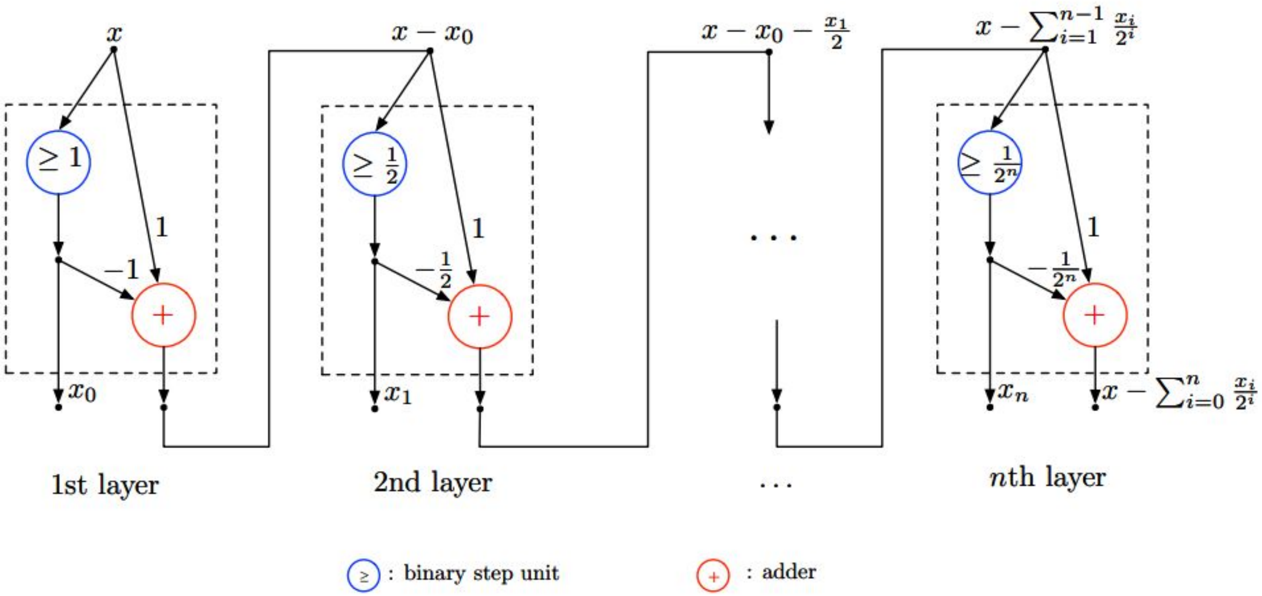
This deep neural network has O (p + log p/ε) layers, O (log p/ε) binary step units and O (p*log p/ε) rectifier linear units.

Theorem 8 of Multivariate Function

Theorem 8. *Let* $W = \{\boldsymbol{w} \in \mathbb{R}^d : \|\boldsymbol{w}\|_1 = 1\}$. *For* $f(\boldsymbol{x}) = \prod_{i=1}^{p} (\boldsymbol{w}_i^T \boldsymbol{x})$, $\boldsymbol{x} \in [0,1]^d$ *and* $\boldsymbol{w}_i \in W$, $i = 1, ..., p$, *there exists a deep neural network* $\tilde{f}(\boldsymbol{x})$ *with* $\mathcal{O}\left(p + \log \frac{pd}{\varepsilon}\right)$ *layers and* $\mathcal{O}\left(\log \frac{pd}{\varepsilon}\right)$ *binary step units and* $\mathcal{O}\left(pd \log \frac{pd}{\varepsilon}\right)$ *rectifier linear units such that* $|f(\boldsymbol{x}) - \tilde{f}(\boldsymbol{x})| \leq \varepsilon$, $\forall \boldsymbol{x} \in [0,1]^d$.

Theorem 8 is for a product of multivariate linear functions.

N bit binary expansion



Universal Approximation Theorem

- According to the Universal Approximation Theorem, Neural Networks has a kind of universality i.e. there is a network that can approximate f(x) no matter what kind of function f(x) is. [3]
- This Universal Approximation Theorem holds even if the neural network has just a single layer and an input and the output layer.
- **Universal approximation theorem** *(L1 distance, ReLU activation, arbitrary depth, minimal width).* For any Bochner–Lebesgue p-integrable function $f : \mathbb{R}^n \to \mathbb{R}^m$ and any $\epsilon > 0$, there exists a fully-connected ReLU network F of width exactly $d_m = \max\{n+1, m\}$, satisfying

$$\int_{\mathbb{R}^n} \|f(x) - F(x)\|^p \mathrm{d}x < \epsilon.$$

Moreover, there exists a function $f \in L^p(\mathbb{R}^n, \mathbb{R}^m)$ and some $\epsilon > 0$, for which there is no fully-connected ReLU network of width less than $d_m = \max\{n+1, m\}$ satisfying the above approximation bound.

Quadratic function

Data:

- 1000 data points, x∈[0,1]
- Binary expansion to $x = \sum_{i=0}^{\infty} \frac{x_i}{2^i}$, where $x_i \in \{0, 1\}$

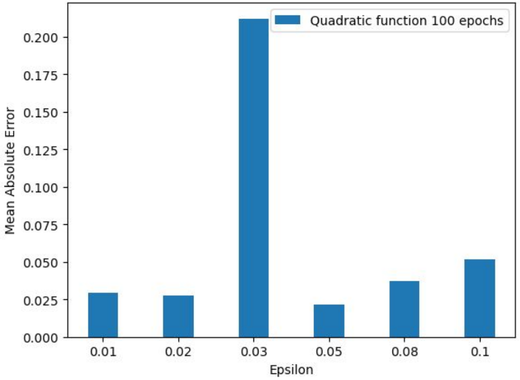
Neural network:

1 input layer of binary step unit, 1 hidden layer of ReLU, 1 output layer

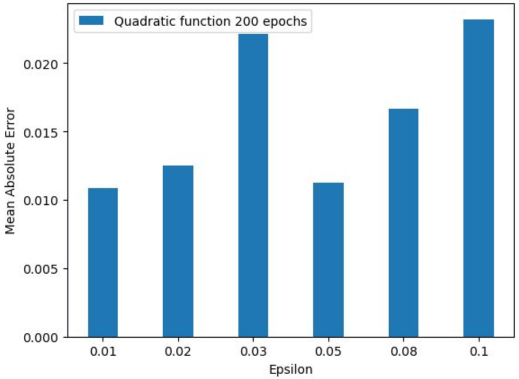
Choose $n = \left\lceil \log_2 \frac{1}{\varepsilon} \right\rceil + 1$

Therefore, the model has $\mathcal{O}\left(\log \frac{1}{\varepsilon}\right)$ layers, $\mathcal{O}\left(\log \frac{1}{\varepsilon}\right)$ binary step units and $\mathcal{O}\left(\log \frac{1}{\varepsilon}\right)$ ReLU

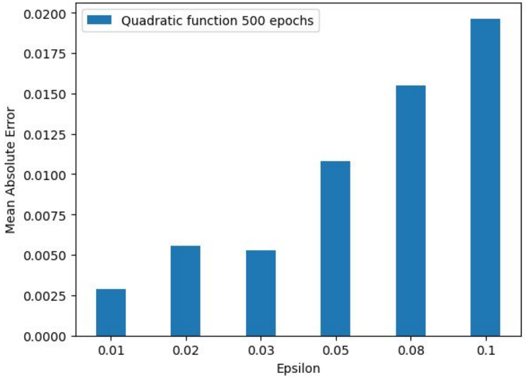
Result for different epsilon and epoches



100 epoches



200 epochs



500 epoches

Polynomial Function Approximation

Data:

- $f(x) = \sum_{i=0}^{p} a_i x^i,\ x \in [0,1]\ and\ \sum_{i=1}^{p} |a_i| \leq 1$
- 1000 data points, x∈[0,1]
- p polynomial coefficients, randomly generated and normalized
- Binary expansion to $x = \sum_{i=0}^{\infty} \frac{x_i}{2^i}$, where $x_i \in \{0, 1\}$

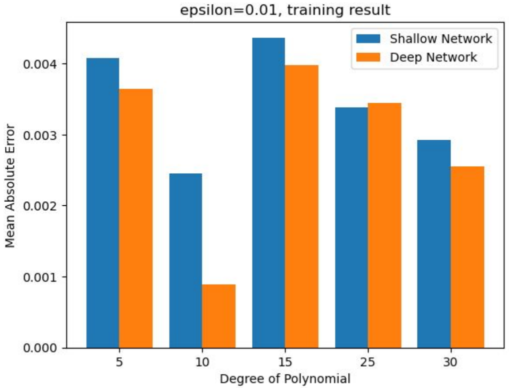
Total number of rectifier linear units = $p \log \frac{p}{\varepsilon}$

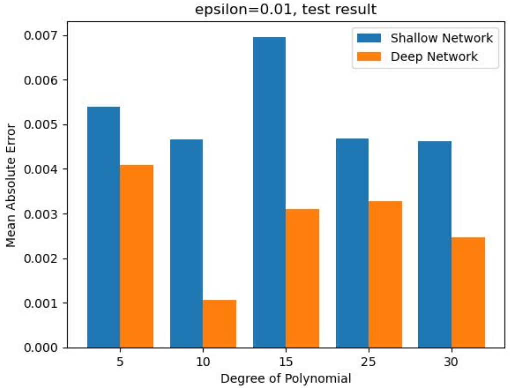
Number of rectifier linear units in each layer = $\log \frac{p}{\varepsilon}$

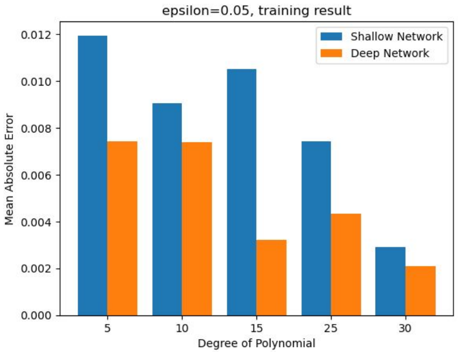
Shallow Neural Network: 1 input layer, 1 hidden layer, 1 output layer

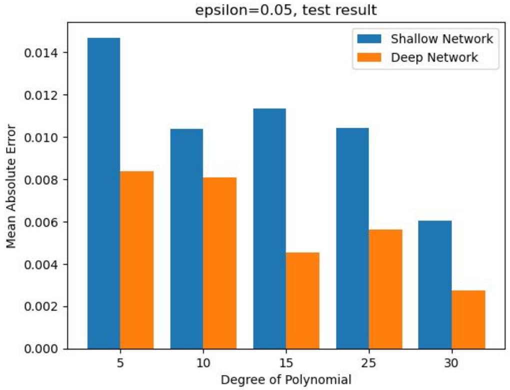
Deep Neural Network: 1 input layer, p hidden layers, 1 output layer

Approximation of Polynomial Functions









Approximation of Multivariate Functions

Data:

- $f(\boldsymbol{x}) = \prod_{i=1}^{p} (\boldsymbol{w}_i^T \boldsymbol{x}),\ \boldsymbol{x} \in [0,1]^d$ *and* $\boldsymbol{w}_i \in W,\ i = 1, \ldots, p,$
- 1000 data points for each pair of (p, d)

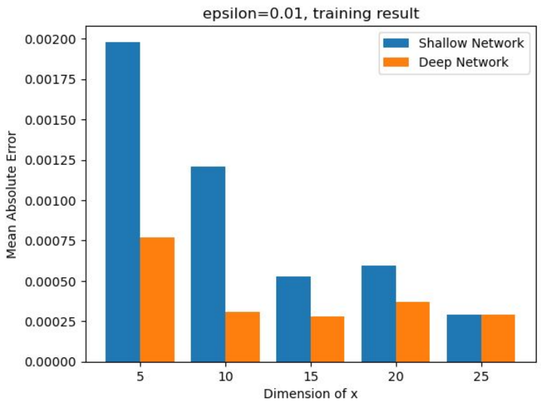
Total Number of rectifier linear units = $pd \log \frac{pd}{\varepsilon}$

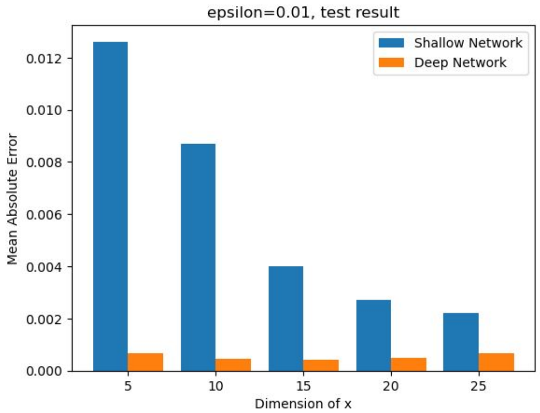
Number of rectifier linear unit in each layer = $d \log \frac{pd}{\varepsilon}$

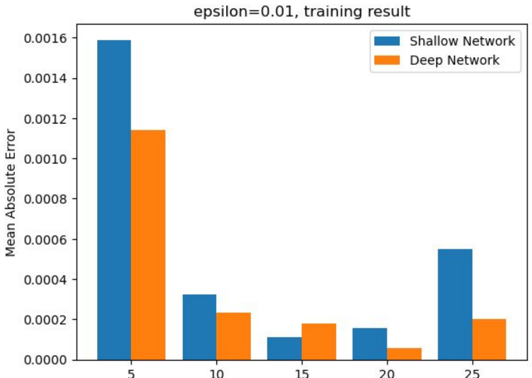
Shallow Neural Network: 1 input layer, 1 hidden layer, 1 output layer

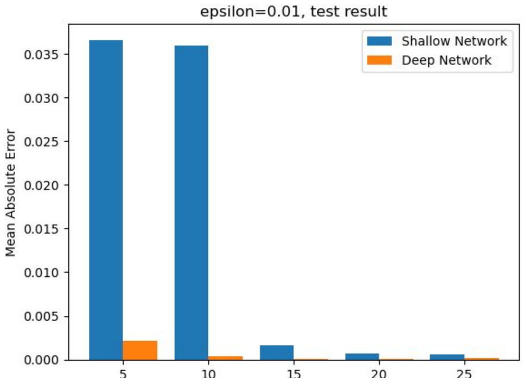
Deep Neural Network: 1 input layer, p hidden layers, 1 output layer

Approximation of Multivariate Functions









Reference

[1] WHY DEEP NEURAL NETWORKS FOR FUNCTION APPROXIMATION?, Liang and Srikant, 2017

[2] https://en.wikipedia.org/wiki/Universal_approximation_theorem

[3] http://neuralnetworksanddeeplearning.com/chap4.html