Deep Approximation via Deep Learning

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Outline

1. Introduction of approximation theory
2. Approximation of functions by compositions
3. Approximation rate in term of number of nurons

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Function $g : \mathbb{R}^n \to \mathbb{R}$ can be as simple as $g(x) = a \cdot x$. To make sense of this approximation, we need to find a map $T : \mathbb{R}^d \mapsto \mathbb{R}^n$, such that

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1. Classical approximation: T is independent of f or data, while n depends on ϵ.
2. Learning: T is learned from data and determined by a few parameters. n depends on ϵ.
3. Deep learning: T is fully learned from data with huge number of parameters. T is a composition of many simple maps, and n can be independent of ϵ.

Classical approximation

- Linear approximation: Given a finite fixed set of generators $\{\phi_1, \ldots, \phi_n\}$, e.g. splines, wavelet frames, finite elements or generators in reproducing kernel Hilbert spaces. Define

  $$T = [\phi_1, \phi_2, \ldots, \phi_n]^\top : \mathbb{R}^d \mapsto \mathbb{R}^n \quad \text{and} \quad g(x) = a \cdot x.$$

  The linear approximation is to find $a \in \mathbb{R}^n$ such that

  $$g \circ T = \sum_{i=1}^{n} a_i \phi_i \sim f$$

  It is linear because $f_1 \sim g_1, f_2 \sim g_2 \Rightarrow f_1 + f_2 \sim g_1 + g_2$.

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- The best n-term approximation: Given dictionary $\mathcal{D}$ that can have infinitely many generators , e.g. $\mathcal{D} = \{\phi_i\}_{i=1}^\infty$ and define

  $$T = [\phi_1, \phi_2, \dots,]^\top : \mathbb{R}^d \mapsto \in \mathbb{R}^\infty \quad \text{and} \quad g(x) = a \cdot x$$

  The best n-term approximation of f is to find a with n nonzero terms such that $g \circ T \sim f$.is the best approximation among all the n-term choices

  It is nonlinear because $f_1 \sim g_1, f_2 \sim g_2 \nRightarrow f_1 + f_2 \sim g_1 + g_2$, as the support of the a_1 and a_2 depends on f_1 and f_2.

Examples

Consider a function space $L_2(\mathbb{R}^d)$, let $\{\phi_i\}_{i=1}^{\infty}$ be an orthonormal basis of $L_2(\mathbb{R}^d)$.

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Linear approximation

For a given n, $T = [\phi_1, \ldots, \phi_n]^\top$ and $g = a \cdot x$ where $a_j = \langle f, \phi_j \rangle$. Denote $\mathcal{H} = \mathrm{span}\{\phi_1, \ldots, \phi_n\} \subseteq L_2(\mathbb{R}^d)$.
Then,

$$g \circ T = \sum_{i=1}^{n} \langle f, \phi_i \rangle \phi_i$$

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is the orthogonal projection onto the space $\mathcal{H}$ and is the best approximation of f from the space $\mathcal{H}$.
$g \circ T$ provides a good approximation of f when the sequence $\{\langle f, \phi_j \rangle\}_{j=1}^{\infty}$ decays fast as $j \to +\infty$.
Therefore,

1. Linear approximation provides a good approximation for smooth functions.
2. **Advantage:** It is a good approximation scheme for d is small, domain is simple, function form is complicated but smooth.
3. **Disadvantage:** It does not do well if d is big and/or domain of f is complex.

Examples

The best n-term approximation

$T = (\phi_j)_{j=1}^{\infty} : \mathbb{R}^d \mapsto \mathbb{R}^{\infty}$ and $g(x) = a \cdot x$ and each a_j is

$$a_j = \begin{cases} \langle f, \phi_j \rangle, & \text{for the largest } n \text{ terms in the sequence } \{|\langle f, \phi_j \rangle|\}_{j=1}^{\infty} \\ 0, & \text{otherwise.} \end{cases}$$

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The approximation of f by $g \circ T$ depends less on the decay of the sequence $\{|\langle f, \phi_j \rangle|\}_{j=1}^{\infty}$. Therefore,

1. the best n-term approximation is better than the linear approximation when f is nonsmooth.
2. It is not a good scheme if d is big and/or domain of f is complex.

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Given data $\{(x_i, f(x_i))\}_{i=1}^m$.

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1. The key of deep learning is to construct a T by the given data and chosen g.
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3. It is robust to approximate f by $g \circ T$.

Classical approximation vs deep learning

For both linear and the best n-term approximations, T is fixed. Neither of them suits for approximating f, when f is defined on a complex domain, e.g manifold in a very high dimensional space.

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What is the mathematics behind this?

Settings: construct a measurable map $T : \mathbb{R}^d \mapsto \mathbb{R}^n$ and a simple function g (e.g. $g = a \cdot x$) from data such that the feature of the domain of f can be rearranged by T to match with those of g. This leads to $g \circ T$ provides a good approximation of f.

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Approximation by compositions (with Qianxiao Li and Cheng Tai)

Question 1: For given f and g, is there a measurable $T : \mathbb{R}^d \mapsto \mathbb{R}^n$ such that $f = g \circ T$?

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Answer: Yes! We have proven

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ *and* $g : \mathbb{R}^n \to \mathbb{R}$ *and assume* $\mathrm{Im}(f) \subseteq \mathrm{Im}(g)$ *and* g *is continuous. Then, there exists a measurable map* $T : \mathbb{R}^d \mapsto \mathbb{R}^n$ *such that*

$$f = g \circ T, \; a.e.$$

- This is an existence proof. T cannot be written out analytically. This leads to the following relaxed question

Approximation by compositions

Question 2: For arbitrarily given $\epsilon > 0$, can one construct a measurable $T : \mathbb{R}^d \mapsto \mathbb{R}^n$ such that $\|f - g \circ T\| \leq \epsilon$?

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Answer: Yes!

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ and $g : \mathbb{R}^n \to \mathbb{R}$ and assume $\mathrm{Im}(f) \subseteq \mathrm{Im}(g)$. For an arbitrarily given $\epsilon > 0$, a measurable map $T : \mathbb{R}^d \mapsto \mathbb{R}^n$ can be constructed in terms of f and g, such that

$$\|f - g \circ T\| \leq \epsilon$$

- While T can be written out in terms of f and g, T can be complex to be constructed when only sample data of f is given. This leads to

Approximation by compositions

Question 3: Can T be a composition of simple maps? That is, can we write $T = T_1 \circ \cdots \circ T_J$, where each T_i, $i = 1, 2, \ldots, J$ is simple, e.g. “perturbation of identity.”

Answer: Yes!

Theorem

Denote $f : \mathbb{R}^d \to \mathbb{R}$ *and* $g : \mathbb{R}^n \to \mathbb{R}$*. For an arbitrarily given* $\epsilon > 0$*, if* $\mathrm{Im}(f) \subseteq \mathrm{Im}(g)$*, then there exists* J *simple maps* $T_i, i = 1, 2, \ldots, J$ *such that* $T = T_1 \circ T_2 \ldots \circ T_J : \mathbb{R}^d \mapsto \mathbb{R}^n$ *and*

$$\|f - g \circ T_1 \circ \cdots \circ T_J\| \leq \epsilon$$

The proof of existence of T_i, $i = 1, 2, \ldots, J$ is constructive. In fact, an algorithm can be devised to carry it out approximately in practice.

Algorithm

Input: Hypothesis spaces: $\mathcal{I}$, $\mathcal{H}$; Loss functions: L, L';
Tolerance: ϵ
Data: $\{x_i, f(x_i)\}_{i=1}^N$
Result: A function f_n that approximates a given f
initialization: Set $f_0 = g$, $\mathrm{Im} g \supset \mathrm{Im} f$;
for j *from* 0 *to* $n-1$ **do**
$I_j = \arg\min_{I \in \mathcal{I}} \quad \frac{1}{N} \sum_{i=1}^N L(I(x_i), \mathbb{1}_{\{|f_j - f| > \epsilon\}}(x_i))$;
$h_j = \arg\min_{h \in \mathcal{H}} \quad \frac{1}{N} \sum_{i=1}^N L'(f(x_i), f_j \circ T_{h,j}(x_i))$
where $T_{h,j}(x) := I_j(x)h(x) + [1 - I_j(x)]x$;
Set $f_{j+1} = f_j \circ T_{h_j,j}$
end

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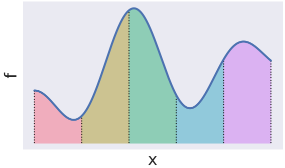
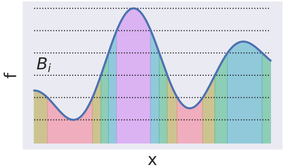
  a, r, p can be estimated at each stage to see if we can go further
- This procedure also naturally picks up some multi-scale structure

Ideas

- Classical approximation sub-divides the domain, The key to a good approximation is to reproduce poly locally. The smoothness of f is needed. It is a local approach (e.g. Riemann integration, TV method).
- Alternative approach sub-divides the range. The key to good approximation is the location, volume, and geometry of $f^{-1}(B_i)$, The smoothness of f is no more important. It is non-local (e.g. Lebesgue integration, non-local TV method)
- Our theory and algorithm iteratively rearranges $f^{-1}(B_i)$ by constructing T, so that it matches with $g^{-1}(B_i)$, Consequently, $g \circ T$ approximates f well.





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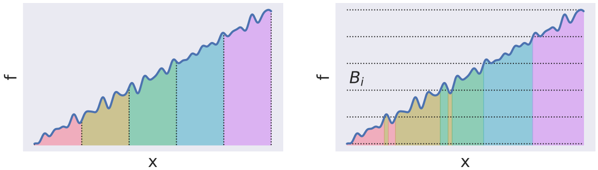
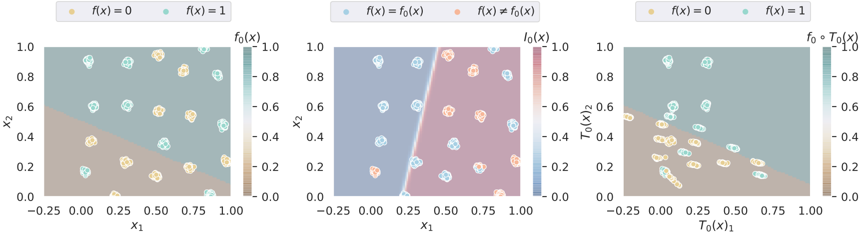
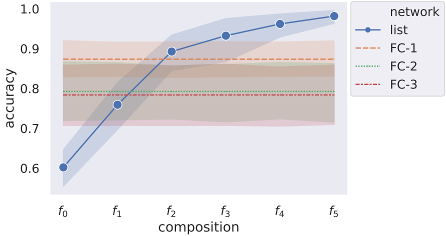
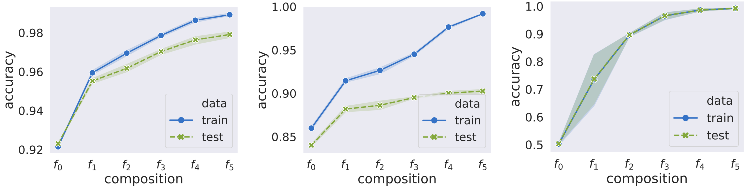


A Binary Classification Toy Problem





Other Classification and Regression Benchmarks



(a) MNIST (b) Fashion-MNIST (c) SGEMM[1]

Remark: For the image classification problems, h, I composes of small convolution blocks with 4-32 channels, and 2-4 layers each. f_0 is linear.

Q. Li, Z. Shen, and C Tai Deep approximation of functions via composition (2019).

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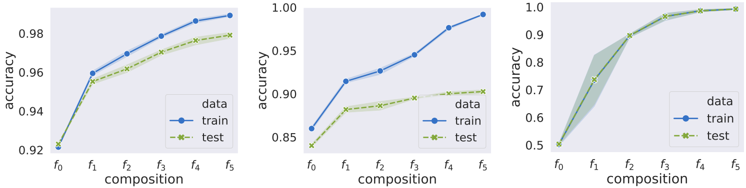

(d) MNIST (e) Fashion-MNIST (f) SGEMM[1]

Remark: The last problem is regression, with fully connected blocks for h, I. "Accuracy" is defined as in the preceding theory: $D_\epsilon(f, f_j) = \mu\{|f - f_j| > \epsilon\}$. Here, we take $\epsilon = 0.1$.

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The best N-term Approximation via Dictionary with Compositions(with Haizhao Yang and Shijun Zhang)

N-term approximation Given a dictionary $\mathcal{D}$ and f, the best

n-term approximation from $\mathcal{D}$ is to find $\phi_i^* \in \mathcal{D}$ and $a_i^* \in \mathbb{R}$ such that

$$g = \sum_{i=1}^{n} a_i^* \phi_i^*$$

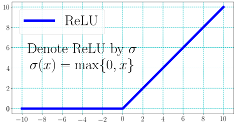
is a solution of

$$\inf_{a_i \in \mathbb{R},\, \phi_i \in \mathcal{D}} \Big\| f - \sum_{i=1}^{n} a_i \phi_i \Big\|.$$

The best N-term Approximation via Dictionary with Compositions

First dictionary is defined as

$$\mathcal{D}_1 := \{\sigma(\boldsymbol{W} \cdot \boldsymbol{x} + b) : \boldsymbol{W} \in \mathbb{R}^d,\, b \in \mathbb{R}\}$$



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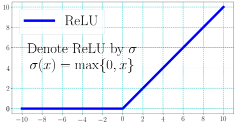

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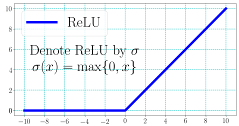

Each element of $\mathcal{D}_1$ is a piecewise linear function.

When $d = 1$, for arbitrary Lipchitz continuous f on $[0, 1]$, the best n-term approximation from $\mathcal{D}_1$ achieve the approximation rate $O(n^{-1})$.

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$$\mathcal{D}_2 \coloneqq \{\sigma(\boldsymbol{W} \cdot \boldsymbol{h} + b) : \boldsymbol{W} \in \mathbb{R}^n,\, b \in \mathbb{R}\}.$$

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Each element of $\mathcal{D}_2$ is compositions of piecewise linear functions.

Compositions of piecewise linear functions are still piecewise linear functions.

This process can continue inductively to derive multilayer composition dictionaries $\mathcal{D}_3, \ldots \mathcal{D}_L$.

The best N-term Approximation via Dictionary with Compositions

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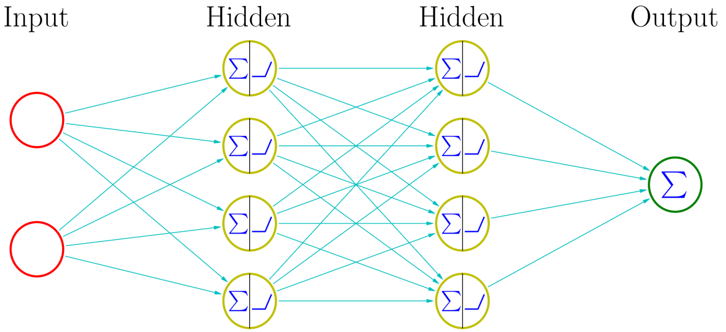

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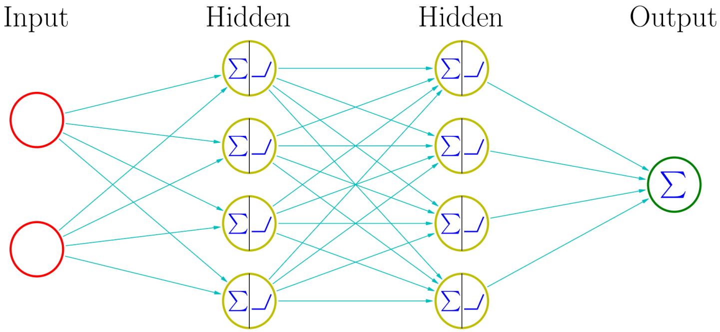

When $d = 1$, for any Lipchitz continuous f on $[0, 1]$, the best n-term approximation from $\mathcal{D}_2$ achieve the approximation rate $O(n^{-2})$.

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dictionary	corresponding network	approximation rate
$\mathcal{D}_1$	1 hidden layer	$O(n^{-1})$
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For any fixed L, can the dictionary $\mathcal{D}_L$ attain the n-term of approximation rate $O(n^{-L})$ for $L \geq 3$?

The answer is unlikely, unless one do something else...

Given $L \geq 1$, there exists f with Lipchitz constant 1 such that the n-term approximation error from $\mathcal{D}_L$ cannot be better than

$$O(n^{-(2+\rho)})$$

for sufficiently large n and any $\rho > 0$.

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How about the case $d > 1$?

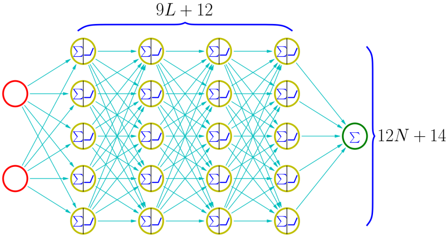
For any Lipchitz continuous f on $[0,1]^d$, the best N-term approximation from the dictionary with composition achieves the approximation rate $O(n^{-2/d})$.

Z. Shen, H. Yang, and S. Zhang, Nonlinear Approximation via Compositions, arXiv e-prints, (2019), arXiv:1902.10170,601p. arXiv:1902.1017.

Approximation Rate of ReLU Networks

For given $N, L > 1 \in \mathbb{N}^+$, design a network of order $O(NL)$

ϕ=



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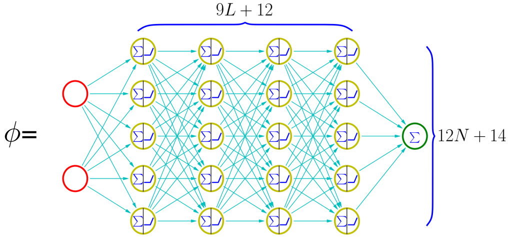

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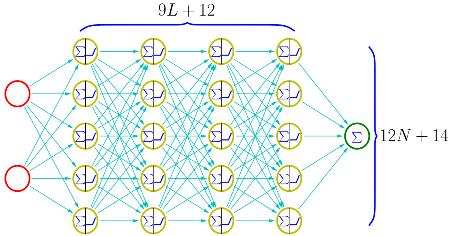
ϕ= 

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Suppose f is Lipchitz with constant ν, then

$$\|f - \phi\|_{L^p([0,1]^d)} \leq 40\nu\sqrt{d}N^{-2/d}L^{-2/d},$$

for $p \in [1, \infty)$.
When $d > 1$, the width is $\max\{8d\lfloor N^{1/d}\rfloor + 4d, 12N + 14\}$.

Approximation Rate of ReLU Networks

For general continuous functions, define the modulus of continuity, for any $r > 0$, as

$$\omega_f(r) := \sup\{|f(\boldsymbol{x}) - f(\boldsymbol{y})| : \boldsymbol{x}, \boldsymbol{y} \in [0,1]^d,\ |\boldsymbol{x} - \boldsymbol{y}| \le r\}.$$

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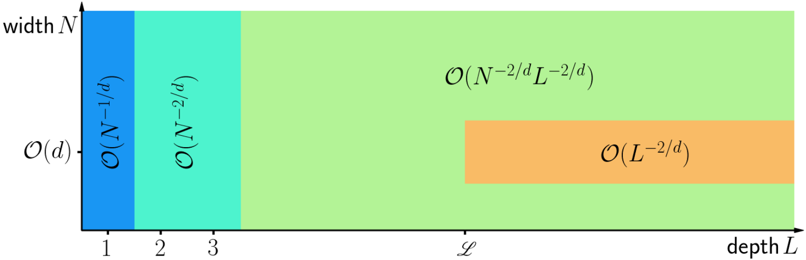
Theorem

Let f be continuous, $\forall\ L > 1, N \in \mathbb{N}^+$ and $\forall\ p \in [1, \infty)$, $\exists$ a ReLU network ϕ with width $\max\left\{8d\lfloor N^{1/d}\rfloor + 4d, 12N + 14\right\}$ and depth $9L + 12$ such that

$$\|f - \phi\|_{L^p([0,1]^d)} \leq 5\omega_f(8\sqrt{d}N^{-2/d}L^{-2/d}).$$

The rate $O(N^{-2/d}L^{-2/d})$ is nearly optimal.

Approximation Rate of ReLU Networks



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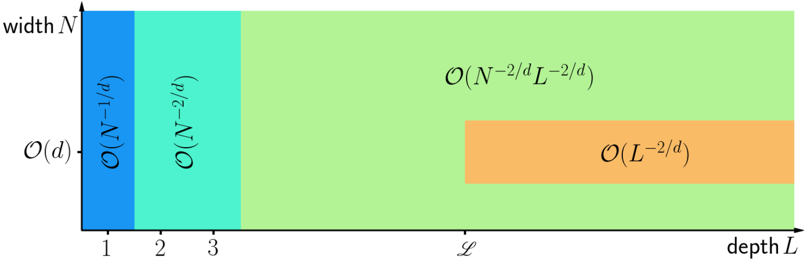

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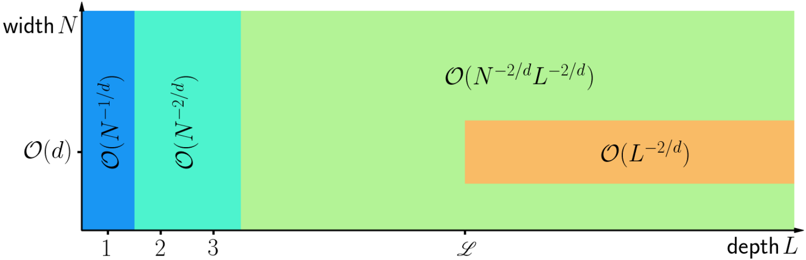

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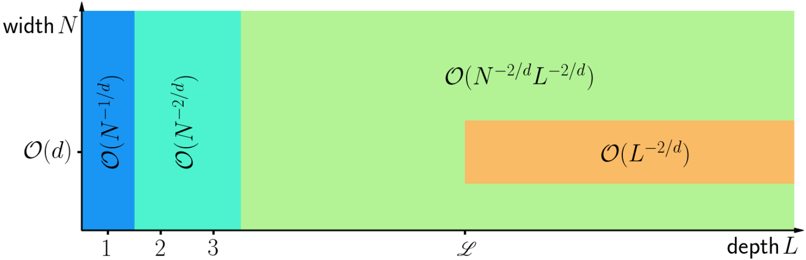

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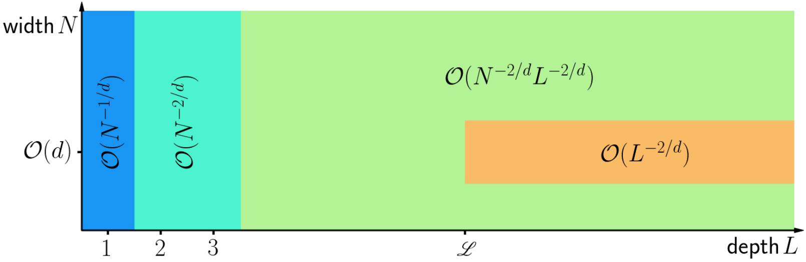

- (blue): $N \geq 1$, $L = 1$, rate $O(N^{-1/d})$, well known.
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- (green): $N \geq 1$, $L \geq 1$, rate $O(N^{-2/d}L^{-2/d})$, Shen, Yang, Zhang, 2019.

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How about the general continuous functions?

We can extend our result to arbitrary continuous functions by using $\omega_f(\cdot)$ as we defined previously.

Approximation on Low-Dimensional Manifold

Define ε-neighborhood of $d_{\mathcal{M}}$-dim manifold $\mathcal{M} \subseteq [0,1]^d$ as

$$\mathcal{M}_\varepsilon := \Big\{ \boldsymbol{x} \in [0,1]^d : \inf\{|\boldsymbol{x} - \boldsymbol{y}| : \boldsymbol{y} \in \mathcal{M}\} \leq \varepsilon \Big\},$$

Let $\varrho(\cdot)$ be a PDF supported on $\mathcal{M}_\varepsilon$ and we say $\mu_\varrho(\cdot)$ is a measure of a probability density function (PDF) $\varrho(\cdot)$ if

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Theorem

Let $f \in C([0,1]^d)$. $\forall$, $N, L \in .\mathbb{N}^+$, and $\epsilon \in (0,1)$, (ϵ can be $O(N^{-2/d_\delta} L^{-2/d_\delta})$), $\exists$ a ReLU network ϕ with width $\max\left\{8d_\delta \lfloor N^{1/d_\delta} \rfloor + 4d_\delta, 12N + 14\right\}$ and depth $9L + 12$ s.t.

$$\|f - \phi\|_{L^p([0,1]^d, \mu_\varrho)} \le 3\omega_f\left(8d\,\varepsilon\right) + 5\omega_f\left(32d\, N^{-2/d_\delta} L^{-2/d_\delta}\right),$$

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Zuowei Shen, Haizhao Yang, Shijun Zhang. Deep Network Approximation Characterized by Number of Neurons. 2019.

Happy Birthday John!

http://www.math.nus.edu.sg/∼matzuows/