Analysis of Neural Network

Jinchao Xu 许进超

Penn State University

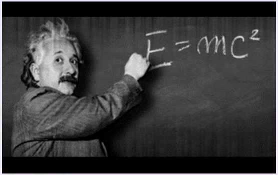
xu@math.psu.edu http://www.math.psu.edu/xu/

CUHK, June 2021

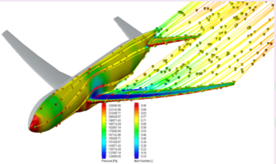
Acknowledgement:
NSF: DMS-1819157

Four major methods of scientific research

Experimental Science



Theoretical Science



Computational Science

Data Science

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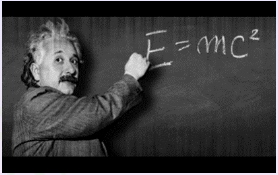

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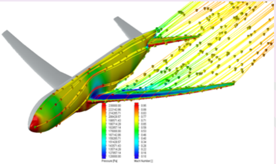

Computational Science

Data Science

Question:

Is “Data Science” really a science?

A basic AI problem: classification

- Can a machine (function) tell the difference ?

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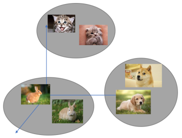

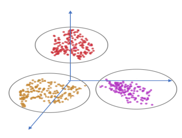

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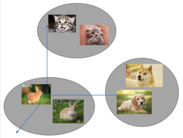

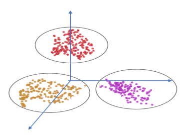

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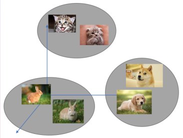

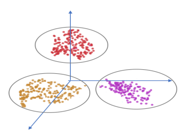

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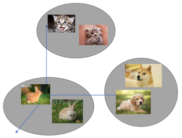

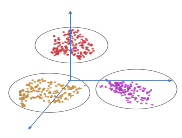

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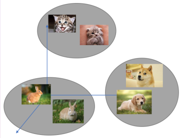

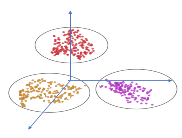

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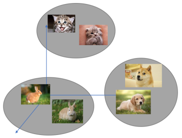

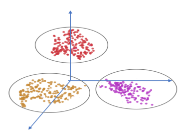

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$$\min_{\Theta} L(x, y, \Theta) \tag{1}$$

where

$$L(x, y, \Theta) = \mathbb{E}_{(x,y)\sim\mathcal{D}}[L(f(x;\Theta), y)] \approx \frac{1}{N}\sum_{i=1}^{N} \|f(x_i;\Theta) - y_i\|^2$$

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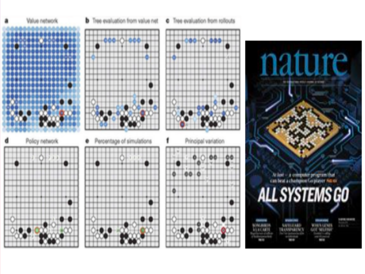
Deep Learning

Machine learning using a special function class:
deep neural networks!

Deep learning and its great successes

CNN has been successfully used in:

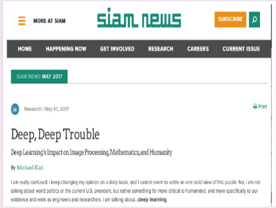
- Computer vision
  - Classification, detection, segmentation...
  - Medical image processing,
  - Face recognition,
- Reinforcement learning
  - AlphaGo,
  - Automated driving,
- Natural language processing
  - Speech recognition,
  - Machine translation,
- ...



Deep Concern

Quotes(Researchers from U Wash, Princeton, MIT, . . .)

- "Deep learning is killing image processing, natural language processing..."
- "Graduate students only work on deep learning"
- "One time extinction event – graduate students won't know the fundamental tools"



Source: D. Donoho/ H. Monajemi/ V. Papyan "Stats 38" at Stanford and B. Dong at PKU

Mathematical understanding and Analysis?

Question:

Why and how do these neural network machine learning models and relevant algorithms work?

Mathematical understanding and Analysis?

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Why and how do these neural network machine learning models and relevant algorithms work?

This series of talks:

1. Finite Element and Deep Neural Network
   - ReLU neural networks $=$ linear finite elements
   - Largest function class that a stable neural network can approximate
   - Optimal approximation rates for popular neural networks
2. Multigrid and Image Classification
   - Linear separable sets and logistic regression
   - A model for feature extractions
   - Image classification by multigrid method
3. Neural Network and Numerical PDEs
   - Error analysis of neural network for numerical PDEs
   - Numerical quadrature and Rademacher complexity analysis
   - Training algorithm that achieves the best asymptotic convergence rate

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For example $n = 100$:

$d =$	2	4	8
$N =$	5×10^3	4.6×10^6	3.5×10^{11}

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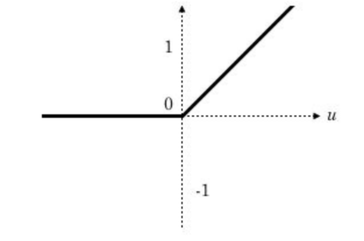
Deep neural network functions with ℓ-hidden layers

$$\Sigma^{\sigma}_{n_{1:\ell}} = \{W^{\ell}x^{(\ell)} + b^{\ell},\ W^i \in \mathbb{R}^{n_i},\ b_i \in \mathbb{R}\}$$

A popular activation function

Ramp or ReLU function

$$\sigma = \mathrm{ReLU}(x) = \max(0, x)$$



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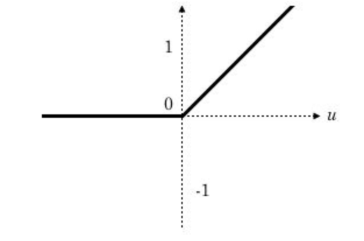

Notation:

$$\Sigma^k_{n_{1:\ell}} = \Sigma^{\mathrm{ReLU}^k}_{n_{1:\ell}}.$$

What does a function in $\Sigma^1_{n_{1:\ell}}$ look like?

Obviously:

$$\Sigma^1_{n_{1:\ell}} = \text{a space of continuous piecewise linear functions!}$$ [1]

[1] **he2018relu**.

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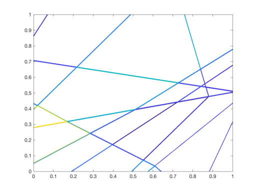
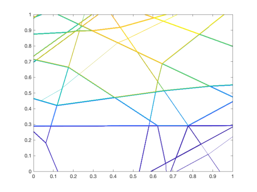
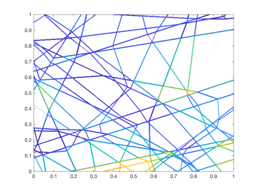


$(10, 10)$



$(20, 20)$



$(40, 40)$

[1] **he2018relu**.

How is $\Sigma^1_{n_{1:\ell}}$ compared with (adaptive) linear FEM?

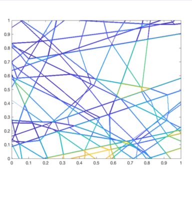


Figure: $(40, 40)$

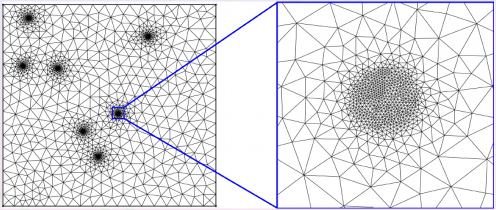


Figure: Adaptive Grid

Finite element: piecewise linear functions

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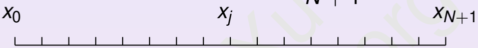
- Uniform grid $\mathcal{T}_h$

$$0 = x_0 < x_1 < \cdots < x_{N+1} = 1, \quad x_j = \frac{j}{N+1} \; (j = 0 : N+1).$$



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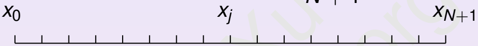
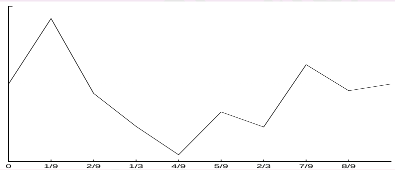
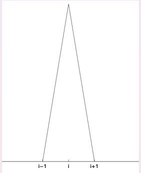


- Linear finite element space

$$V_h = \{ v : \ v \text{ is continuous and piecewise linear w.r.t. } \mathcal{T}_h \}.$$

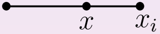


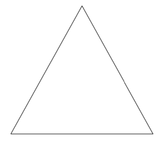


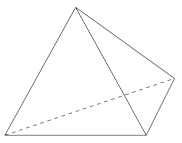
$$v_h(x) = \sum_{i=1}^{n} v_h(x_i)\phi_i(x).$$

Linear finite element in multi-dimensions

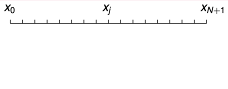
$w_1 x + b$ $\qquad$ $w_1 x_1 + w_2 x_2 + b$ $\qquad$ $w_1 x_1 + w_2 x_2 + w_3 x_3 + b$ $\qquad \cdots$

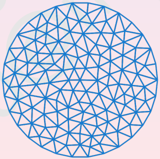


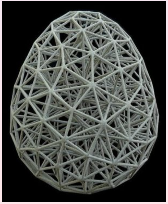




$\cdots$





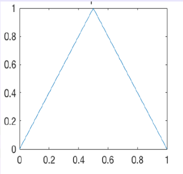


$\cdots$

FEM basis function in 1D

- Denote the basis function in $\mathcal{T}_1$

$$\varphi(x) = \begin{cases} 2x & x \in [0, \frac{1}{2}] \\ 2(1-x) & x \in [\frac{1}{2}, 1] \\ 0, & \text{others} \end{cases}. \qquad (2)$$



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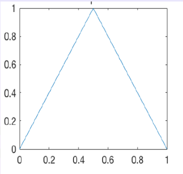
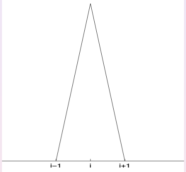
with $w_h = \frac{1}{2h}$, $\quad b_i = \frac{-(i-1)}{2}$.





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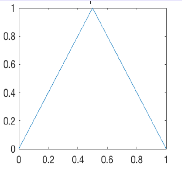
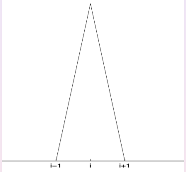
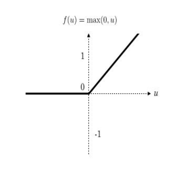
- Let $x_+ = \max(0, x) = \mathrm{ReLU}(x)$,

$$\varphi(x) = 2x_+ - 4(x - 1/2)_+ + 2(x - 1)_+.$$

- $\varphi_i \in \mathrm{span}\left\{(wx + b)_+, w, b \in \mathbb{R}^1\right\}$







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Σ_n^1 is one hidden layer “shallow” neural network with activation function ReLU, n neurons.

Generalization to multi-dimension:

Higher dimension $d \geq 1$

$$\Sigma_n^1 = \left\{ \sum_{i=1}^{n} a_i (w_i x + b_i)_+ : w_i \in \mathbb{R}^{1\times d}, b_i \in \mathbb{R} \right\} \tag{4}$$

where $w_i x = \sum_{j=1}^{d} w_{ij} x_j$.

Connection of ReLU-DNN and Linear FEM

1. $d = 1$,

$$\mathrm{FE} \subset \Sigma_n^1.$$

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3. $d \geq 2$[3],
$$\mathrm{FE} \subset \Sigma_{n_{1:\ell}}^1 \quad \text{for some } \ell > 1,$$
where $\Sigma_{n_{1:\ell}}^1$ is ReLU-DNN with ℓ layers.

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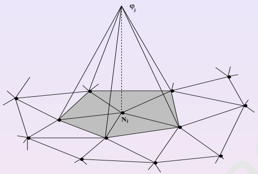
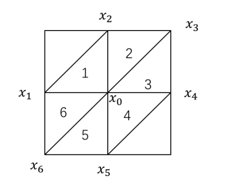
A 2D example: FE basis function

Consider a 2D FE basis function, $\phi(x)$:





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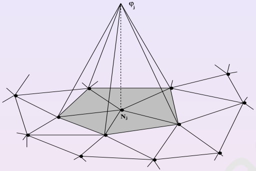

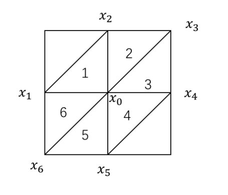

Here g_i is linear in Domain i, and $x_7 = x_1$, satisfying

$$g_i(x_0) = 1 \qquad g_i(x_i) = 0 \qquad g_i(x_{i+1}) = 0$$

$$\phi(x) = \begin{cases} g_i(x), & x \in \text{Domain } i \\ 0. & x \in \mathbb{R}^2 - \overline{x_1 x_2 x_3 x_4 x_5 x_6} \end{cases} \tag{5}$$

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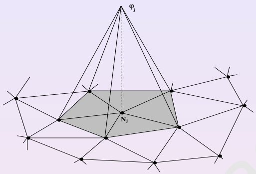

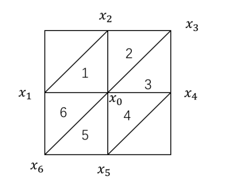

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We have[4][5]

$$\phi \in \Sigma^1_{n_{1:4}}. \tag{6}$$

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We can write the basis function $\phi(x)$ defined on hexagon $\overline{x_1 x_2 x_3 x_4 x_5 x_6}$ which is satisfied that important identities:

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where

$$v = \frac{1}{2}[1, -1, -1, -1] \qquad W = \begin{bmatrix} 1 & 1 \\ -1 & -1 \\ 1 & -1 \\ -1 & 1 \end{bmatrix}$$

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Example of DNN and FEM: 2D-FEM basis function

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g \equiv & \min(g_1, g_2, g_3, g_4, g_5, g_6) = \min(\min(g_1, g_2, g_3), \min(g_4, g_5, g_6)) \\
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$$

ReLU-DNN and Linear FEM for H^1

$$\textit{ReLU-DNN} = \Sigma^1_{n_{1:\ell}}$$

ReLU-DNN and Linear FEM for H^1

$$\textit{ReLU-DNN} = \Sigma^1_{n_{1:\ell}} = \textit{Linear FEM} \subset H^1(\Omega)$$

Shallow Neural Networks

- Superpositions of *ridge functions*

$$\Sigma_n^\sigma := \left\{ \sum_{i=1}^{n} a_i \sigma(\omega_i \cdot x + b_i),\ a_i \in \mathbb{R},\ \omega_i \in \mathbb{R}^d,\ b_i \in \mathbb{R} \right\}$$

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- Shallow networks means one hidden layer, i.e.

$$\Sigma_{[1]}^\sigma = \bigcup_{n=1}^{\infty} \Sigma_n^\sigma \tag{8}$$

Shallow Neural Networks

- Superpositions of *ridge functions*

$$\Sigma_n^\sigma := \left\{ \sum_{i=1}^{n} a_i \sigma(\omega_i \cdot x + b_i),\ a_i \in \mathbb{R},\ \omega_i \in \mathbb{R}^d,\ b_i \in \mathbb{R} \right\}$$

- Shallow networks means one hidden layer, i.e.

$$\Sigma_{[1]}^\sigma = \bigcup_{n=1}^{\infty} \Sigma_n^\sigma \tag{8}$$

- Let $\Omega \subset \mathbb{R}^d$ be a bounded domain

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- Let $\Omega \subset \mathbb{R}^d$ be a bounded domain
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- Consider two problems:
  - Density of $\Sigma_{[1]}^\sigma$ in $L^2(\Omega)$
  - Approximation rates in $L^2(\Omega)$

Are Shallow Networks Dense?

Can shallow networks approximate arbitrary functions?

- Is $\Sigma^{\sigma}_{[1]}$ dense in $L^2(\Omega)$?

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- Is $\Sigma_{[1]}^{\sigma}$ dense in $L^2(\Omega)$?
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- If σ is a polynomial, No!
- Yes! As long as $\sigma \in C^k$ is not a polynomial[6].

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Non-polynomial activation function $\Leftrightarrow$ approximation

Lemma

$\Sigma^{\sigma}_{[1]}$ *is dense in* $C^0(\Omega) \iff \sigma$ *is not a polynomial.*

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- $[\sigma((\omega + he_j) \cdot x + b) - \sigma(\omega \cdot x + b)]/h \in \Sigma^{\sigma}_{[1]}$,

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- $\overline{\Sigma_{[1]}^{\sigma}}$ contains all polynomials.

□

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We note that, for any w_i, b_i

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if $\{w_i\}$ are pairwise linearly independent.

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$$\Sigma^{\sigma}_{[1:k]} \subset \overline{\Sigma^{\sigma}_{[1:k+1]}} \tag{9}$$
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  - Note that we don't always have $\Sigma^{\sigma}_{[1:k]} \subset \Sigma^{\sigma}_{[1:k+1]}$
- How efficiently can functions be approximated?
  - No control of the size of the network or parameters
  - Want approximation rates for networks with controlled weights

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Lemma

For any $g \in L^\infty(G)$, we have

$$\mathbb{E}_n\left(\mathbb{E}g - \frac{1}{n}\sum_{i=1}^n g(\omega_i)\right)^2 = \frac{1}{n}\left(\mathbb{E}(g^2) - (\mathbb{E}(g))^2\right) \le \frac{1}{n}\mathbb{E}(g^2). \tag{12}$$

Sampling Argument

1. Let $u = \int_G g(\omega, x)\lambda(x)dx$ and the sampling $u_n = \frac{1}{n}\sum_{i=1}^{n} g(\omega_i, x)$

$$u(x) - u_n(x) = \mathbb{E}g(x) - \frac{1}{n}\sum_{i=1}^{n} g(\omega_i, x); \tag{13}$$

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3. There exist $\{\omega_i^*\}_{i=1}^n$ such that $u_n = \frac{1}{n}\sum_{i=1}^n g(\omega_i^*, x)$ satisfies

$$\|u - u_n\|_0 \le n^{-\frac{1}{2}} \quad \text{or} \quad \|\mathbb{E}g - \frac{1}{n}\sum_{i=1}^{n} g(\omega_i, x)\|_0 \le n^{-\frac{1}{2}}. \tag{15}$$

Approximation Rates for Cosine Networks

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- Cosine networks

$$\Sigma_n^{\cos} = \left\{ u_n : u_n = \sum_{i=1}^{n} a_i \cos(w_i x + b_i), \quad \forall a_i, w_i, b_i \right\}$$

- Integral representation of u in terms of cosine functions

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Approximation Rates for Cosine Networks[7]

[7] **jones1992simple**.

Approximation Rates for Cosine Networks[7]

1. The preceeding *sampling argument* gives the *approximation rate*:

Theorem

There exists $u_n \in \Sigma^{\cos}_{n,M} = \left\{ \sum_{i=1}^{n} a_i \cos(\omega_i \cdot x + b_i), \sum_{i=1}^{n} |a_i| \leq M \right\}$ *such that*

$$\|u - u_n\| \lesssim n^{-\frac{1}{2}} \|\hat{u}\|_{L^1(\mathbb{R}^d)}.$$

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Spectral Barron Norm

Generalization:

$$\inf_{u_n \in \Sigma_{n,M}^{\cos}} \|u - u_n\|_{H^m(\Omega)} \lesssim n^{-\frac{1}{2}} \|u\|_{B^m(\Omega)}$$

where $B^m(\Omega)$ is the spectral Barron space.

$$\|u\|_{B^m(\Omega)} = \inf_{u_e|_\Omega = u} \int_{\mathbb{R}^d} (1 + |\omega|)^m |\hat{u}_e(\omega)| d\omega$$

Approximation Rates for the ReLU^k Network

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Note that

$$u(x) - \sum_{|\alpha|\leq k} \frac{1}{\alpha!} D^\alpha u(0) x^\alpha = \|\rho\|_{L^1(G)} \int_G g(x,\theta)\lambda(\theta) d\theta = \|\rho\|_{L^1(G)} \mathbb{E}(g)$$

with $\theta = (z, t, \omega) \in G = \{-1, 1\} \times [0, T] \times \mathbb{R}^d$,

$$\rho(\theta) = \frac{1}{(2\pi)^d} |s(zt, \omega)| |\hat{u}(\omega)| \|\omega\|^{k+1}$$

$$s(zt, \omega) = \begin{cases} (-1)^{\frac{k+1}{2}} \cos(z\|\omega\|t + b(\omega)) & k \text{ is odd}, \\ (-1)^{\frac{k+2}{2}} \sin(z\|\omega\|t + b(\omega)) & k \text{ is even}. \end{cases} \quad (16)$$

$$g(x, \theta) = (z\bar{\omega} \cdot x - t)_+^k \,\mathrm{sgn}\, s(zt, \omega), \qquad \lambda(\theta) = \frac{\rho(\theta)}{\|\rho\|_{L^1(G)}}. \quad (17)$$

Approximation Rates for the ReLU^k[8][9]

Lemma (Sampling Analysis)

There exist ω_i, t_i such that

$$\|u - u_n\|_{H^m} \lesssim n^{-\frac{1}{2}} \|u\|_{B^{m+k+1}} \tag{18}$$

with $u_n = \sum_{|\alpha| \leq k} \frac{1}{\alpha!} D^\alpha u(0) x^\alpha + \frac{c}{k!n} \sum_{i=1}^{n} \beta_i (\omega_i \cdot x - t_i)_+^k$.

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Lemma (More Refined Analysis: Stratified Method)

There exist ω_i, t_i *such that*

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with $\bar{\omega}_i = \frac{\omega_i}{\|\omega_i\|}$ *and* $u_n = \sum_{|\alpha| \le k} \frac{1}{\alpha!} D^\alpha u(0) x^\alpha + \frac{c}{k!n} \sum_{i=1}^n \beta_i (\bar{\omega}_i \cdot x - t_i)_+^k$.

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More General Activation Functions

- Using similar techniques, we can extend these rates to more general activation functions as well[10]

Theorem

Suppose that $\sigma \in L^\infty$ *and satisfies the decay condition*

$$|\sigma(t)| \lesssim (1 + |t|)^p \tag{20}$$

for some $p > 1$. *Let* $u \in L^2(\Omega)$. *Then we have*

$$\inf_{u_n \in \Sigma_n^\sigma} \|u - u_n\|_{L^2(\Omega)} \lesssim \|u\|_{B^1(\Omega)} n^{-\frac{1}{2}}. \tag{21}$$

[10] **siegel2020approximation**.

More General Activation Functions (cont.)

- At the cost of a worse rate, we can even drop almost all assumptions on[11] σ

Theorem

Suppose that $\sigma \in L^\infty$ and $\hat{\sigma}$ is continuous and non-zero at a single point. Let $u \in L^2(\Omega)$. Then we have

$$\inf_{u_n \in \Sigma_n^\sigma} \|u - u_n\|_{L^2(\Omega)} \lesssim \|u\|_{B^1(\Omega)} n^{-\frac{1}{4}}. \tag{22}$$

- In particular:
  - Holds for all $\sigma \in L^1 \cap L^\infty$
  - Holds for all $\sigma \in BV$

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Stable Neural Network Approximation

- Recall: approximation of cosine neural network from the function class (by sampling argument):

$$\Sigma_{n,M}^{\cos} = \left\{ \sum_{i=1}^{n} a_i \cos(\omega_i \cdot x + b_i), \sum_{i=1}^{n} |a_i| \leq M, \quad M = \|\hat{u}\|_{L^1} \right\}$$

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- How far can the sampling argument go?
- Consider approximation from the class

$$\Sigma^{\sigma}_{n,M} := \left\{ \sum_{i=1}^{n} a_i \sigma(\omega_i \cdot x + b_i), \ \omega_i \in \mathbb{R}^d, \ b_i \in \mathbb{R}, \sum_{i=1}^{n} |a_i| \le M \right\} \tag{23}$$

of neural networks with ℓ^1-bounded outer coefficients.

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of neural networks with ℓ^1-bounded outer coefficients.
- More generally for a dictionary $\mathbb{D} \subset H = L^2(\Omega)$, consider

$$\Sigma_{n,M}(\mathbb{D}) = \left\{ \sum_{i=1}^{n} a_i h_i,\ h_i \in \mathbb{D},\ \sum_{i=1}^{n} |a_i| \le M \right\} \tag{24}$$

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- Let $M < \infty$ be fixed and consider approximation as $n \to \infty$.

Stable Dictionary Approximation Space

Siegel & Xu, 2021[12]:

- Define a closed convex hull of $\pm\mathbb{D}$:

$$B_1(\mathbb{D}) = \overline{\cup_{n=1}^{\infty} \Sigma_{n,1}^{\sigma}}, \tag{25}$$

[12] **siegel2021optimal**.

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- Define a closed convex hull of $\pm\mathbb{D}$:

$$B_1(\mathbb{D}) = \overline{\cup_{n=1}^{\infty} \Sigma_{n,1}^{\sigma}}, \tag{25}$$

- Define a norm

$$\|f\|_{\mathcal{K}_1(\mathbb{D})} = \inf\{r > 0 : f \in rB_1(\mathbb{D})\}, \tag{26}$$

as the guage of the set $B_1(\mathbb{D})$.

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Stable Dictionary Approximation Space

Siegel & Xu, 2021[12]:

- Define a closed convex hull of $\pm\mathbb{D}$:

$$B_1(\mathbb{D}) = \overline{\cup_{n=1}^{\infty}\Sigma_{n,1}^{\sigma}}, \tag{25}$$

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$$\{f \in H : \|f\|_{\mathcal{K}_1(\mathbb{D})} < \infty\} = \cup_{M>0}\overline{\cup_{n=1}^{\infty}\Sigma_{n,M}^{\sigma}} \tag{28}$$

  is a Banach space.

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- Thus the norm is given by

$$\mathcal{K}_1(\mathbb{D}) = \ell^1 \subset \ell^2. \tag{30}$$

Stable Dictionary Approximation Space

Theorem (Siegel & Xu 2021)

A function $f \in H = L^2(\Omega)$ can be approximated at all, i.e.

$$\lim_{n\to\infty} \inf_{f_n \in \Sigma_{n,M}(\mathbb{D})} \|f - f_n\|_H = 0, \tag{31}$$

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Furthermore, if

$$\|\mathbb{D}\| \equiv \sup_{h\in\mathbb{D}} \|h\|_H < \infty$$

we have

$$\inf_{f_n \in \Sigma_{n,M}(\mathbb{D})} \|f - f_n\|_H \le n^{-\frac{1}{2}} \|\mathbb{D}\| \|f\|_{\mathcal{K}_1(\mathbb{D})}. \tag{32}$$

The Spectral Barron Space

- Let $f \in B_1(\mathbb{D})$, $H = L^2(\Omega)$, $\Omega = B_1^d = \{x \in \mathbb{R}^d : |x| \leq 1\}$, and

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- Property:

$$H^{s+\frac{d}{2}+\varepsilon}(\Omega) \hookrightarrow B^s(\Omega) \hookrightarrow W^{s,\infty}(\Omega). \tag{35}$$

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The results are proved in Siegel and Xu 2021[14]

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- We have$\mathcal{K}_1(\mathbb{P}_k^d) \supset \mathcal{K}_1(\mathbb{F}_{k+1}^d)$ (for $k = 0$, Barron 1993[16])

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Previous Best Results

For some dictionaries $\mathbb{D}$, the $n^{-\frac{1}{2}}$ approximation rate can be improved!

- For $\mathbb{D} = \mathbb{P}_0^d$, we have[17]

$$\sup_{f \in B_1(\mathbb{D})} \inf_{f_n \in \Sigma_{n,M}} \|f - f_n\|_{L^2(B_1^d)} \lesssim n^{-\frac{1}{2} - \frac{1}{2d}}. \tag{37}$$

- For $\mathbb{D} = \mathbb{P}_k^d$ for $k \geq 1$, we have[18],[19], if f is in some spectral Barron space:

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- What are the optimal approximation rates?

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New Optimal Bounds

We have the optimal approximation rates[20]

Theorem

For $\mathbb{D} = \mathbb{P}_k^d$ for $k \geq 1$, we have

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In comparison: optimal bound for finite elements[21]

Theorem

Assume that V_h^k is a finite element of degree k on quasi-uniform mesh $\{\mathcal{T}_h\}$ of $\mathcal{O}(N)$ elements. Assume u is sufficiently smooth and not piecewise polynomials, then we have

$$c(u)n^{-\frac{k}{d}} \leq \inf_{v_h \in V_h^k} \|u - v_h\|_{L^2(\Omega)} \leq C(u)n^{-\frac{k}{d}} = \mathcal{O}(h^k). \tag{40}$$

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Removing the constraint that $\sum_{i=1}^{n} |a_i| \leq M$

Define

$$\Sigma_n^k := \left\{ \sum_{i=1}^{n} a_i \sigma_k(\omega_i \cdot x + b_i),\ \omega_i \in \mathbb{R}^d,\ b_i \in \mathbb{R}, a_i \in \mathbb{R} \right\}. \quad (41)$$

Then Σ_n^k has the following approximation property[22]

Theorem (Siegel and Xu)

$$\inf_{f_n \in \Sigma_n^k} \|f - f_n\| \lesssim \begin{cases} n^{-\frac{1}{2}} & \|f\|_{\mathcal{K}_1(\mathbb{F}_s^d)} \quad \text{if} \quad s = \frac{1}{2} \\ n^{-(k+1)} \log n & \|f\|_{\mathcal{K}_1(\mathbb{F}_s^d)} \quad \text{for some} \quad s > 1 \end{cases} \quad (42)$$

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- Improves result of Barron[23] by relaxing condition on f
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- Comparison with FEM:

$$\inf_{w \in \Sigma_n^k} \|u - w\| \approx \left\{ \inf_{v \in V_n^k} \|u - v\| \right\}^{d}.$$

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Thank you!