A Corrective View of Neural Networks: Representation, Memorization and Learning

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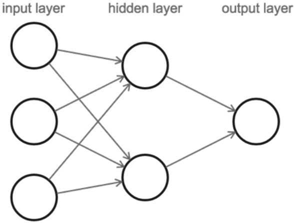
Joint work with Guy Bresler

Overview

Introduction

Neural Networks are universal approximators[1]. We introduce a mathematical tool to obtain

- Sharp bounds on the number of neurons required for representation



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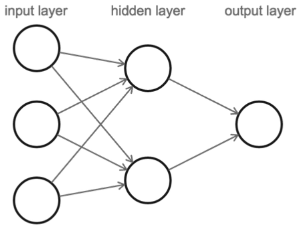

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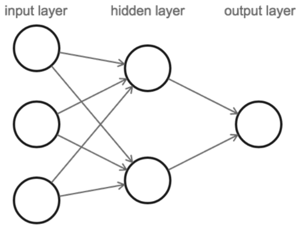
Neural Networks are universal approximators[1]. We introduce a mathematical tool to obtain

- Sharp bounds on the number of neurons required for representation
- State of the art memorization results
- Subpolynomial bounds on number of neurons required to learn low-degree polynomials via. SGD/GD



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Our Results - Memorization

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- Long line of papers aims to understand memorization in over-parametrized networks via the study of SGD/GD

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  Two-layer ReLU networks require $\tilde{O}(\frac{n}{\theta^4} \log \frac{1}{\epsilon})$ non-linear units
- Near optimal in n for two layer ReLU networks and first work to achieve this via. GD

Our Results - Memorization

Work	Assumption	Guarantee	Remarks
Allen-Zhu, Li, and Song 2018	Minimum distance θ	$O(\frac{n^{24}d}{\theta^8})$	
Du et al. 2019	Distinct points	$O(n^6)$	extra factors
Ji and Telgarsky 2019	NTK separability Minimum distance θ	$\log(n)$ $O(\frac{n^{24}}{\theta^8})$	
Oymak and Soltanolkotabi 2019	$d \leq n \leq cd^2$, data i.i.d unif$(\mathcal{S}^{d-1})$	$O(\frac{n^2}{d})$	w.h.p over data
Song and Yang 2019	Distinct points	$O(n^4)$	extra factors
Daniely 2019	$n = d^c$, i.i.d unif$(\mathcal{S}^{d-1})$	$\tilde{O}(n/d)$	w.h.p over data
Kawaguchi and Huang 2019	Minimum distance θ	$\tilde{O}(n)$	
Our Work	Minimum distance θ	$\tilde{O}(\frac{n}{\theta^4})$	

Table: Comparison of Guarantees for number of non-linear units

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- We can replace d with effective dimension $q \ll d$ when there is 'low-dimensional structure'. Ex: low-degree polynomials.

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- Our results show that we can do the same with a two-layer network

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- First sub-polynomial learning bounds

Corrective Mechanism - The Main Idea

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- Under certain conditions, ‘a’ corrective steps give a rate of $1/N^a$.

Representation to Learning: Random Features Model

- 2 layer network (one linear, one non-linear):

$$\hat{f}(x) = \sum_{i=1}^{N} \kappa_i \mathrm{ReLU}(\langle w_i, x \rangle - T_i)$$

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- SGD for neural networks with a large number of neurons reduces to this approximately.

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- The 'random features' optimization must give κ_i^* which can do better than κ_i^0 (error of at most 'ϵ')

Memorization - Proof

- Data : $\{(x_1, y_1), \ldots, (x_n, y_n)\}$. Construct discrete Fourier transform:

$$F(\xi) = \sum_{j=1}^{n} y_j e^{i\langle \xi, x_j \rangle} .$$

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- $\xi \sim \mathcal{N}(0, \sigma^2 I_d)$, $\sigma \sim \frac{\sqrt{\log n}}{\theta}$, $\theta =$ min. distance.
- 'Inverse Fourier tranform':

$$\begin{aligned} y_j &\approx \mathbb{E} F(\xi) e^{-i\langle \xi, x_j \rangle} \\ &= \mathbb{E}|F(\xi)| \cos(\langle \xi, x_j \rangle + \psi(\xi)) \end{aligned} \tag{1}$$

Memorization - Proof

- 'Cosine Representation' : cos function as integrals of ReLU. Let $T \sim \text{unif}[-2,2]$, independent of ξ.

$$y_j \approx \mathbb{E}C(1+\tilde{O}(1/\theta^2))|F(\xi)|\eta(T,\xi)\mathrm{ReLU}\left(\frac{\langle \xi, x_j\rangle}{\omega_0} - T\right) \tag{2}$$

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- Contruct empirical estimator: $(\xi_k, T_k) \sim \mathcal{N}(0,\sigma^2 I_d) \times \text{Unif}[-2,2]$ i.i.d:

$$\hat{y}_j^{(1)} = \frac{1}{N_0}\sum_{k=1}^{N_0} C(1+\tilde{O}(1/\theta^2))|F(\xi_k)|\eta(T_k,\xi_k)\mathrm{ReLU}\left(\frac{\langle \xi_k, x_j\rangle}{\omega_0} - T_k\right).$$

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- Contraction in ℓ^2 via Gaussian concentration:

$$\mathbb{E}\|\mathbf{y}-\hat{\mathbf{y}}^{(1)}\|_2^2 \leq \tilde{O}(\tfrac{n}{\theta^4 N_0})\|\mathbf{y}\|_2^2$$

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- Continue $l = O(\log \frac{n}{\epsilon})$ times:

$$\mathbb{E}\|\mathbf{y} - \sum_{s=1}^{l} \hat{\mathbf{y}}^{(s)}\| \leq \left[\tilde{O}(\tfrac{n}{\theta^4 N_0})\right]^l \|\mathbf{y}\|_2^2 \leq \epsilon \, .$$

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- We conclude that memorization requires $\tilde{O}(\frac{n}{\theta^4} \log \frac{1}{\epsilon})$ activation functions.

Representation Theorems

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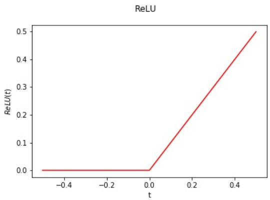
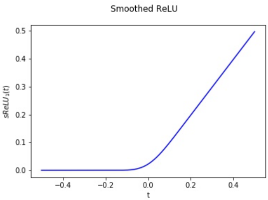
- Uses a mixture of ReLU and smoothed ReLU (SReLU_k) activation functions. SReLU_k are same as ReLU outside a neighborhood of 0 and are $2k$ times continuously differentiable.



(a) ReLU



(b) SReLU_1

Figure: Illustrating ReLU and SReLU activation functions.

Representation Theorems

- Approximate target function f by $\hat{f}^{(1)}$ (two layer SReLU_k network) with N activation functions.

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  Where C_f is a norm on the Fourier transform of f.[3]
- Fourier transform of $\hat{f}^{(1)}$ is an unbiased estimator for the Fourier tranform of f. Therefore, (roughly)

$$C_{f-\hat{f}^{(1)}} \leq C\frac{C_f}{\sqrt{N}}\,.$$

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Representation Theorems

- Let $f^{\text{rem}} := f - \hat{f}^{(1)}$. We can approximate f^{rem} by $\hat{f}^{(2)}$ with N non-linear units such that:

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- Therefore, $\hat{f}^{(1)} + \hat{f}^{(2)}$ approximates f up to an error of $\frac{1}{N^2}$. We can continue this 'a' times to get rates of $\frac{1}{N^a}$.
- After each corrective step, the remainder function becomes less and less smooth till further approximation is impossible (depending on how smooth the original function is).

- Consider $f(x) = \sum_V J_V p_V(x)$ - degree q multinomial over $\mathbb{R}^d$.

[4] Andoni et al. 2014; Yehudai and Shamir 2019.

[5] Liang and Srikant 2016; Safran and Shamir 2017; Yarotsky 2017.

Application : Learning Low-degree Polynomials

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- **Our results for learning:** $O(d^{q(1+\delta)}\text{subpoly}_q(1/\epsilon))$ ($\delta \to 0$ as $\epsilon \to 0$). Gives us the first sub-polynomial learning guarantees.

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- $f(x)$ effective dimension $q << d$. It is infinitely differentiable - so we can achieve rates of $\frac{C(a,q)}{N^a}$ for arbitrary $a \in \mathbb{N}$.
- Sample ω_i and T_i from a tractable distribution, there exist coefficients b_i such that the random neural network

$$\hat{f}(x; \mathbf{b}) = \sum_{i=1}^{N} b_i \mathrm{SReLU}_{j_i}\left(\frac{\langle \omega_i, x \rangle}{\sqrt{q}} - T_i\right)$$

approximates f up to a squared error of $C(a,q)\frac{d^{q(a+1)}}{N^a}$ in expectation

- Whenever $N \geq C(a, q)d^{q\frac{a+1}{a}}(\epsilon\delta)^{-\frac{1}{a}}$, with probability atleast $1-\delta$ (over the randomness in the weights), we can pick coefficients $b_{i,j,V}$ so that squared error is at most ϵ.

Learning Low-degree Polynomials

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- Let $a \to \infty$ slowly enough as $\epsilon \to 0$. This gives us subpolynomial bounds.

Thank You