Learning with norm-based neural networks: model capacity, function spaces, and computational-statistical gaps

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[joint work with Leello Dadi, Zhenyu Zhu, Volkan Cevher (EPFL)]

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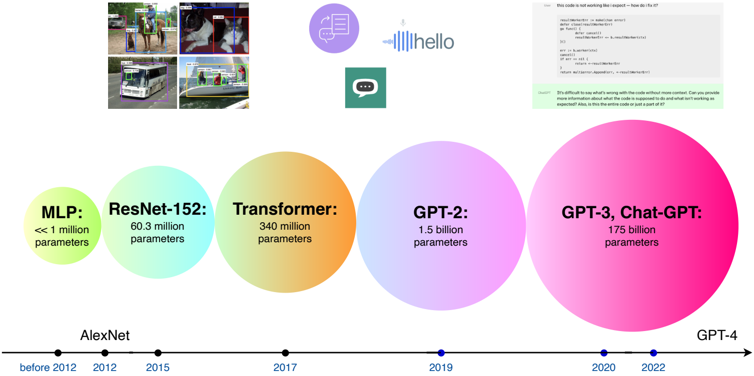
Over-parameterization: more parameters than training data



Scaling law: under compute budget

scaling law [14]

test loss = A $\times$ Model Size^{-a} + B $\times$ Data Size^{-b} + C

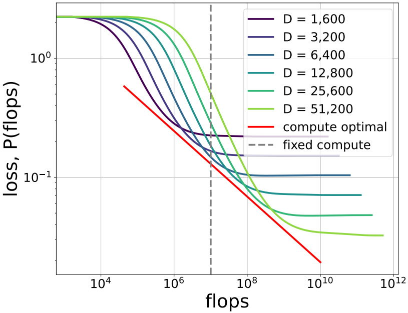
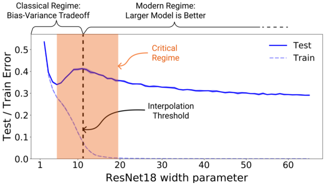


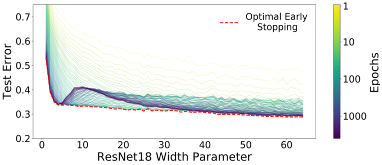
Figure 1: Scaling law under compute-optimal configuration [21].

Model size is a “right” complexity?

- double descent [6] (Belkin, Hsu, Ma, Mandal, 2019)



(a) Results on ResNet18 [18]



(b) Optimal early stopping [18].

- Empirically: neural network pruning [16], lottery ticket hypothesis [12], fine-tuning with large dropout [27]
- Theoretically: how much over-parameterization is sufficient? [8, 25]

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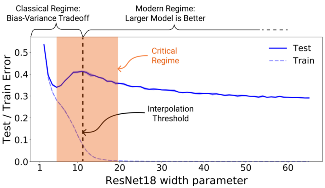

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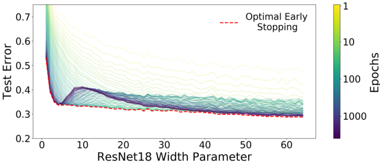

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What is the “right” model complexity?

◦ Complexity of a prediction rule, e.g.,

- number of parameters
- norm of parameters

[3] (Bartlett, 1998)

The size of the weights is more important than the size of the network!

Norm-based capacity:[19, 23, 20, 9]

name	definition	rank correlation
Parameter Frobenius norm	$\sum_{i=1}^{L} \|W_i\|_F^2$	0.073
Frobenius distance to initialization [17]	$\sum_{i=1}^{L} \|W_i - W_i^0\|_F^2$	−0.263
Spectral complexity [4]	$\prod_{i=1}^{L} \|W_i\| \left(\sum_{i=1}^{L} \frac{\|W_i\|_{2,1}^{3/2}}{\|W_i\|^{3/2}}\right)^{2/3}$	−0.537
Fisher-Rao [15]	$\frac{(L+1)^2}{n} \sum_{i=1}^{n} \langle W, \nabla_W \ell(h_W(x_i), y_i) \rangle$	0.078
Path-norm [19]	$\sum_{(i_0,\dots,i_L)} \prod_{j=1}^{L} \left(W_{i_j, i_{j-1}}\right)^2$	0.373

Table 1: Complexity measures compared in the empirical study [13], and their correlation with generalization

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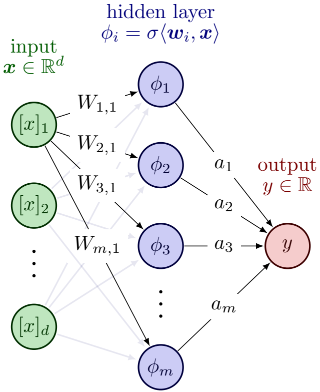
$$\mathcal{P}_m = \left\{ f_{\boldsymbol{\theta}}(\cdot) := \frac{1}{m} \sum_{k=1}^{m} a_k \phi\big(\langle \boldsymbol{w}_k, \cdot \rangle\big) \right\}$$



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ℓ_1-path norm

$$\|\boldsymbol{\theta}\|_{\mathcal{P}} := \frac{1}{m} \sum_{k=1}^{m} |a_k| \|\boldsymbol{w}_k\|_1$$

- equivalent to Barron spaces [2, 11]

$$\mathcal{B} := \cup_{\mu \in \mathcal{P}(\mathcal{W})} \{ f_a : \|\boldsymbol{a}\|_{L^2(\mu)} < \infty \}$$

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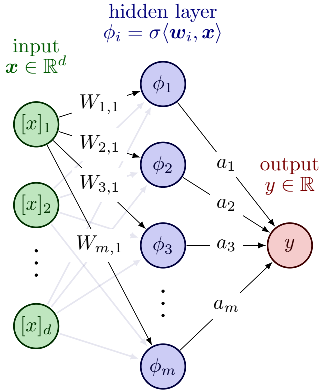

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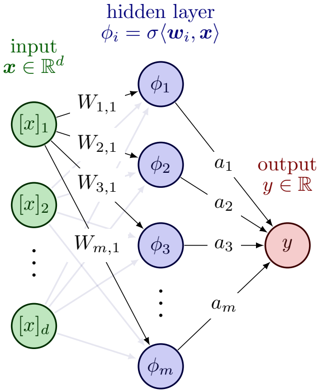

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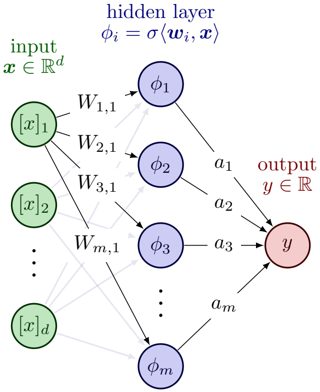

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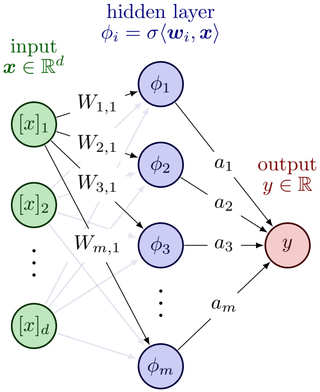

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Our results: statistical guarantees

For the class of two-layer neural networks $\mathcal{G}_R = \{f_{\boldsymbol{\theta}} \in \mathcal{P}_m : \|\boldsymbol{\theta}\|_{\mathcal{P}} \leqslant R\}$

$$\widehat{f_{\boldsymbol{\theta}}} := \operatorname*{argmin}_{f_{\boldsymbol{\theta}} \in \mathcal{G}_R} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_{\boldsymbol{\theta}}(\boldsymbol{x}_i))^2 \,.$$

Theorem (Liu, Dadi, Cevher, JMLR 2024)

Under standard assumptions (bounded data, $f^\star \in \mathcal{B}$), for two-layer over-parameterized neural networks, we have

$$\left\|\widehat{f_{\theta}} - f^\star\right\|^2_{L^2_{\rho_X}} \lesssim \frac{R^2}{m} + R^2 d^{\frac{1}{3}} n^{-\frac{d+2}{2d+2}} \qquad w.h.p.$$

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Sample complexity

Proposition (metric entropy)

For bounded data $\|\boldsymbol{x}\|_\infty \leq 1$*, denote* $\mathcal{G}_R = \{f_{\boldsymbol{\theta}} \in \mathcal{P}_m : \|\boldsymbol{\theta}\|_{\mathcal{P}} \leqslant R\}$*, the metric entropy of* $\mathcal{G}_1$ *can be bounded by*

$$\log \mathcal{N}_2(\mathcal{G}_1, \epsilon) \leqslant Cd\epsilon^{-\frac{2d}{d+2}}\,, \quad \forall \epsilon > 0 \quad \textit{and} \quad d \geq 5\,,$$

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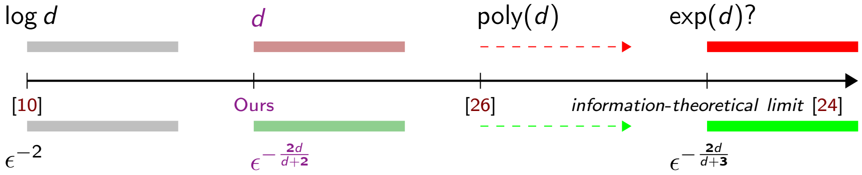

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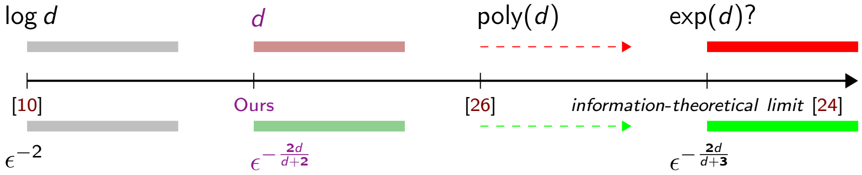

The "best" trade-off between ϵ and d.

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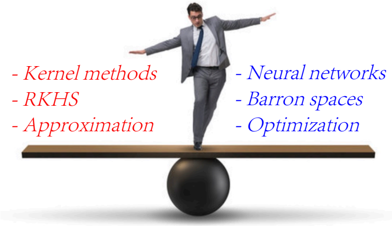

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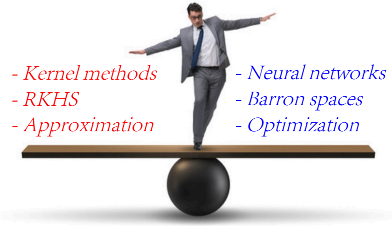

Do some Barron functions can be learned by two-layer NNs, both statistically and computationally efficient?

Learning with multiple ReLU neurons under GD training

Can we learn multiple ReLU neurons by two-layer NNs, both statistically and computationally efficient?

$$f^\star(\boldsymbol{x}) = \sum_{l=1}^{k} \sigma(\langle \boldsymbol{v}_l, \boldsymbol{x} \rangle), k = \mathcal{O}(1)$$

$\|\hat{f} - f^\star\|_{L^2(\mathrm{d}\mu)} \leq \epsilon$ from $\{\boldsymbol{x}_i, f^\star(\boldsymbol{x}_i)\}_{i=1}^n$ with $\boldsymbol{x}_i \sim \mathcal{N}(0, \boldsymbol{I}_d)$

Theorem ([7] PAC learning $f^\star$ under Gaussian measure)

There exists an algorithm that requires time/samples at $(d/\epsilon)^{\mathcal{O}(k^2)}$

- correlational statistical query (CSQ): $|\tilde{q} - \mathbb{E}_{\boldsymbol{x},y}[\psi(\boldsymbol{x})y]| \leq \tau$

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Assumption

- *diverse teacher neurons:* $\{\boldsymbol{v}_l\}_{l=1}^{d}$ *are (nearly) orthogonal and* $\|\boldsymbol{v}_l\|_2 = \texttt{const}$
- *warm start: the smallest angle not close to orthogonal*
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$$L(\boldsymbol{W}) = \frac{1}{2}\mathbb{E}_{\boldsymbol{x}\sim\mathcal{N}(0,\boldsymbol{I}_d)}\left(\sum_{i=1}^{m}\sigma(\langle \boldsymbol{w}_i, \boldsymbol{x}\rangle) - \sum_{l=1}^{k}\sigma(\langle \boldsymbol{v}_l, \boldsymbol{x}\rangle)\right)^2$$

- Gaussian initialization $\boldsymbol{w}_i \sim \mathcal{N}(0, \sigma^2 \boldsymbol{I}_d)$
- angle: $\theta_{il} \triangleq \angle(\boldsymbol{w}_i, \boldsymbol{v}_l)$

Assumption

- *diverse teacher neurons:* $\{\boldsymbol{v}_l\}_{l=1}^d$ *are (nearly) orthogonal and* $\|\boldsymbol{v}_l\|_2 = \texttt{const}$
- *warm start: the smallest angle not close to orthogonal*
  - *hold w.p.* $\exp(-\mathcal{O}(1))$ *for fixed dimension*

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Theorem (Zhu, Liu, Cevher, 2024)

For sufficiently small initialization and step-size $\sigma, \eta = o(m^{-k^2})$, *then there exists a time* $T_2 = \frac{1}{\eta}$ *such that* $\forall T \in \mathbb{N}$ *and* $i \in [m]$,

$$L(\boldsymbol{W}(T + T_2)) \leq \mathcal{O}\left(\frac{1}{T^3}\right), \|\boldsymbol{w}_i(T + T_2)\|_2 = \Theta\left(\frac{k\|\boldsymbol{v}\|_2}{m}\right) \; w.h.p.$$

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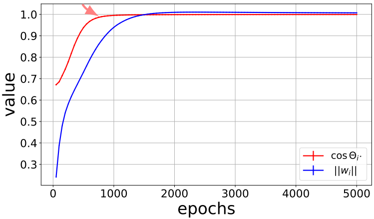
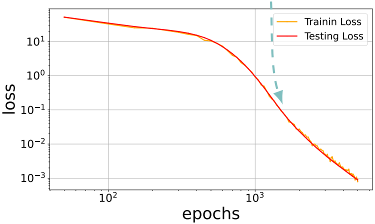
- align $\theta_{i^*} \to 0$ norm converge then fit





Take-away messages

- model size -> size of weights -> path norm -> Barron spaces
- statistical guarantees with improved sample complexity
- computational-statistical gap -> learning with multiple ReLU neurons

We're organizing one workshop at NeurIPS 2024!

Fine-Tuning in Modern Machine Learning: Principles and Scalability

https://sites.google.com/view/neurips2024-ftw/home

Thanks for your attention!

Q & A

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Background: RFMs and kernel methods

Consider a RFM with infinite many features $f_a(\boldsymbol{x}) = \int_{\mathcal{W}} a(\boldsymbol{w})\phi(\boldsymbol{x}, \boldsymbol{w})\mathrm{d}\mu(\boldsymbol{w})$, define

$$\mathcal{F}_{p,\mu} := \{f_a : \|\boldsymbol{a}\|_{L^p(\mu)} < \infty\}, \quad \|f\|_{\mathcal{F}_{p,\mu}} := \inf_{f_a = f} \|\boldsymbol{a}\|_{L^p(\mu)}$$

- RFMs $\equiv$ kernel methods by taking $p = 2$ using Representer theorem [22]
  - function space: reproducing kernel Hilbert space $\mathcal{H}_{k_\mu} = \mathcal{F}_{2,\mu}$

$$\hat{k}_m(\boldsymbol{x}, \boldsymbol{x}') = \frac{1}{m}\sum_{i=1}^{m} \phi(\boldsymbol{x}, \boldsymbol{w}_i)\phi(\boldsymbol{x}', \boldsymbol{w}_i) \rightarrow k_\mu(\boldsymbol{x}, \boldsymbol{x}') = \int_{\mathcal{W}} \phi(\boldsymbol{x}, \boldsymbol{w})\phi(\boldsymbol{x}', \boldsymbol{w})\mathrm{d}\mu(\boldsymbol{w})$$

- RFMs $\not\equiv$ kernel methods if $p < 2$

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From RKHS to Barron space

Definition (Barron space [11] (E, Ma, Wu, 2021))

For any $1 \leq p \leq \infty$, we have

$$\mathcal{B} = \cup_{\mu \in \mathcal{P}(\mathcal{W})} \mathcal{F}_{p,\mu}\,, \quad \|f\|_{\mathcal{B}} = \inf_{\mu \in \mathcal{P}(\mathcal{W})} \|f\|_{\mathcal{F}_{p,\mu}}$$

Remark: ◦ Two-layer neural networks: data-adaptive kernel $\mathcal{B} = \cup_{\mu \in \mathcal{P}(\mathcal{W})} \mathcal{H}_{k_\mu}$

◦ equivalent to path norm $\|\Theta\|_{\mathcal{P}} := \frac{1}{m}\sum_{k=1}^{m} |a_k| \|\boldsymbol{w}_k\|_1$

◦ parameter space vs. measure space

e.g., [1] (Bach, 2017), [5] (Bartolucci, Vito, Rosasco, Vigogna, 2022).

Optimization in Barron spaces is difficult: curse of dimensionality!

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