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

Fanghui Liu

fanghui.liu@warwick.ac.uk

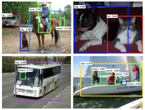
Department of Computer Science, University of Warwick, UK

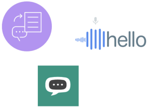
Centre for Discrete Mathematics and its Applications (DIMAP), Warwick

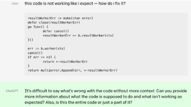
[joint work with Leello Dadi, Zhenyu Zhu, Volkan Cevher (EPFL)]

at Department of Computer Science, University of Wisconsin-Madison

In the era of deep learning



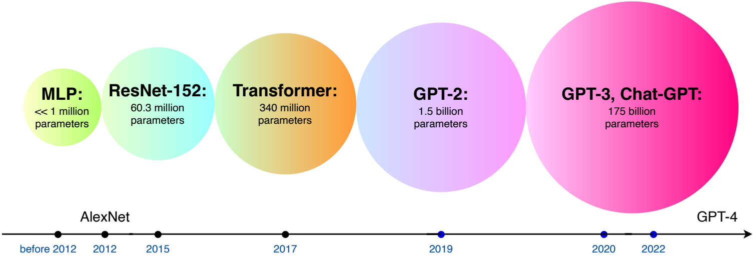



User this code is not working like i expect — how do i fix it?

```
resultWorkerErr := make(chan error)
defer close(resultWorkerErr)
go func() {
        defer cancel()
        resultWorkerErr <- b.resultWorker(ctx)
}()

err := b.worker(ctx)
cancel()
if err == nil {
        return <-resultWorkerErr
}
return multierror.Append(err, <-resultWorkerErr)
```

ChatGPT It's difficult to say what's wrong with the code without more context. Can you provide more information about what the code is supposed to do and what isn't working as expected? Also, is this the entire code or just a part of it?



Learning paradigm transition in the past twenty years

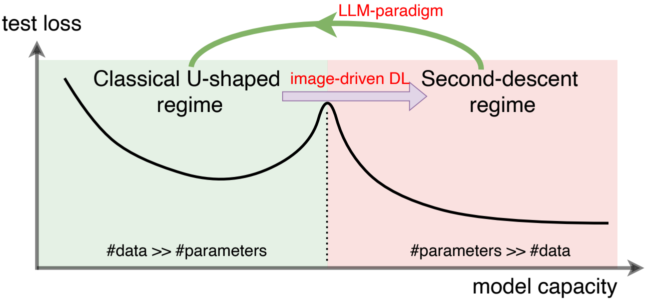


Figure 1: Paradigm among test loss, data, and model capacity.

- double descent [5] (Belkin, Hsu, Ma, Mandal, 2019)

scaling law [15]

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

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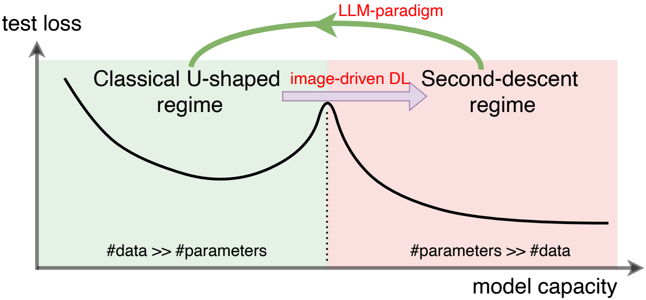

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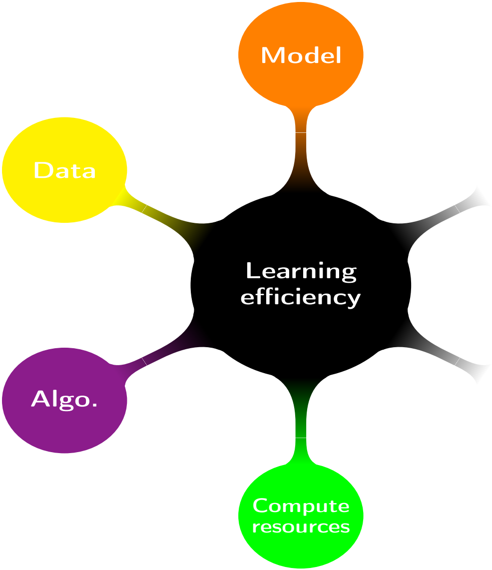
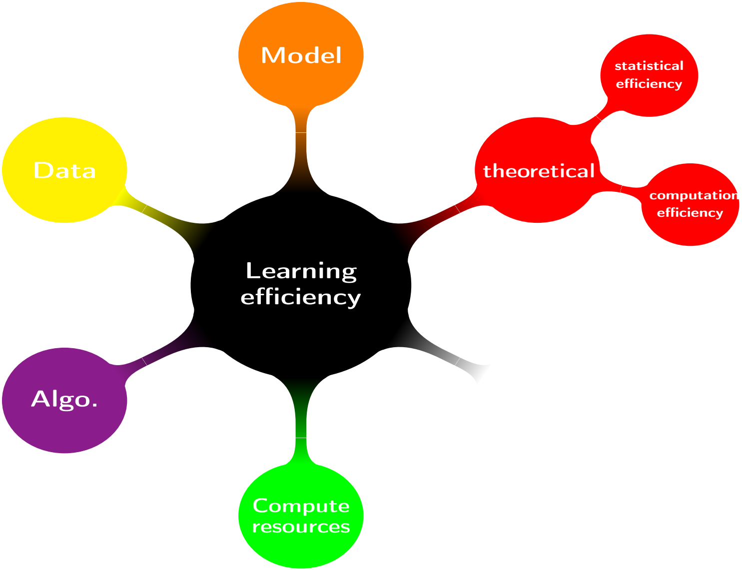
Pipeline: Learning efficiency - curse of dimensionality



Pipeline: Learning efficiency - Theory



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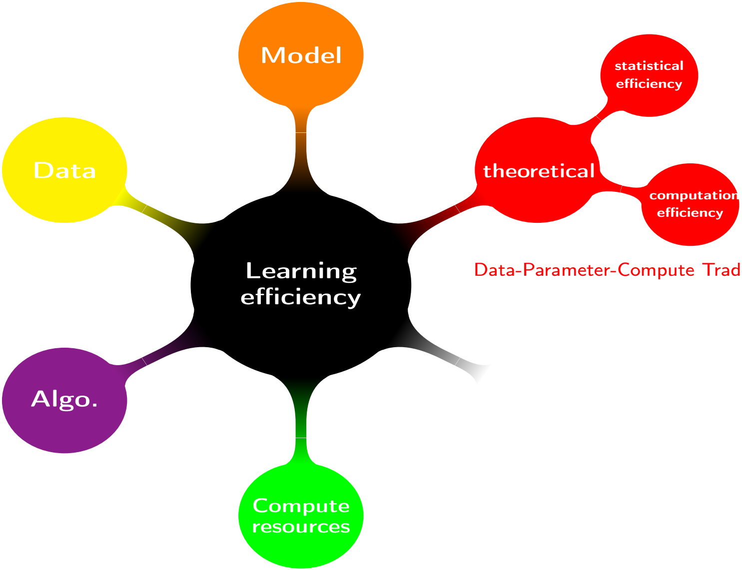
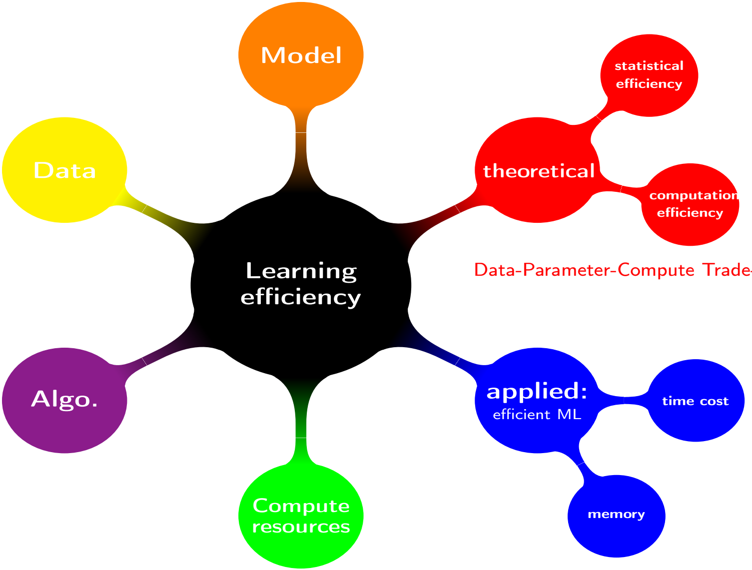


Data-Parameter-Compute Trade-offs!

Pipeline: Learning efficiency - Application



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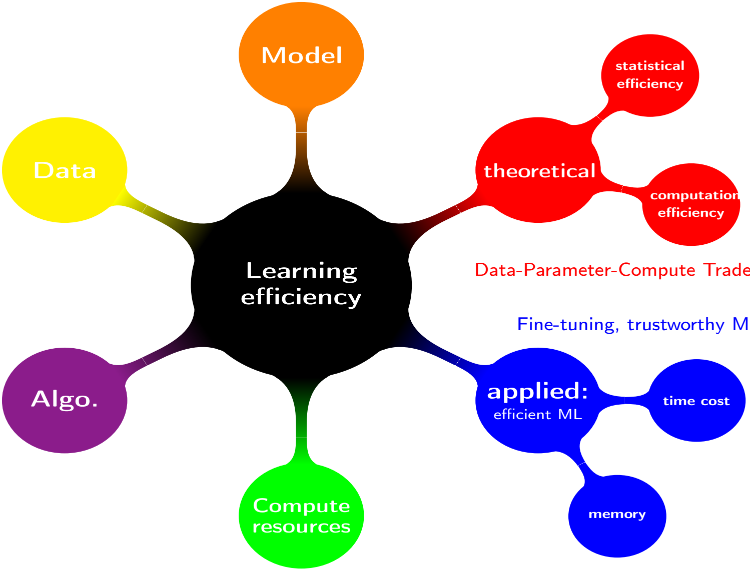

Data-Parameter-Compute Trade-offs!

Fine-tuning, trustworthy ML etc

Outline

- model size is a good metric?
- Learning with path-norm: the perspective of model capacity
- Learning with Barron spaces: the perspective of function space
- statistical/computational learning efficiency

Target

Characterize the "right" model capacity as well as the induced "right" *function spaces* for ML models and track statistical/computational learning efficiency.

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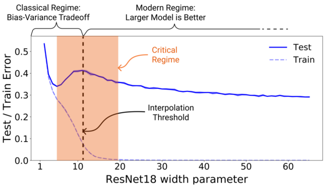
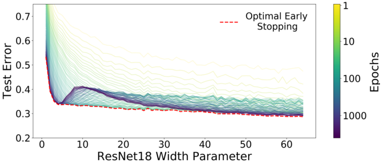
- double descent can disappear!



(a) Results on ResNet18 [20]



(b) Optimal early stopping [20].

- Empirically: neural network pruning [18], lottery ticket hypothesis [13], fine-tuning with large dropout [31]
- Theoretically: how much over-parameterization is sufficient [8, 28]

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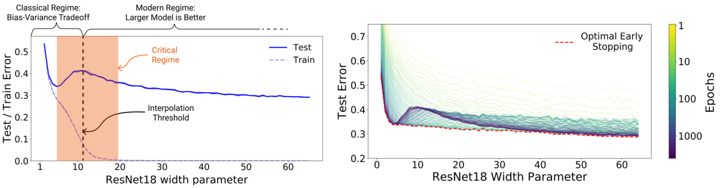

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What is the "right" model complexity?

◦ 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:[21, 25, 22, 10]

name	definition	rank correlation
Parameter Frobenius norm	$\sum_{i=1}^{L} \|\boldsymbol{W}_i\|_F^2$	0.073
Frobenius distance to initialization [19]	$\sum_{i=1}^{L} \|\boldsymbol{W}_i - \boldsymbol{W}_i^0\|_{\mathrm{F}}^2$	−0.263
Spectral complexity [4]	$\prod_{i=1}^{L} \|\boldsymbol{W}_i\| \left(\sum_{i=1}^{L} \frac{\|\boldsymbol{W}_i\|_{2,1}^{3/2}}{\|\boldsymbol{W}_i\|^{3/2}}\right)^{2/3}$	−0.537
Fisher-Rao [16]	$\frac{(L+1)^2}{n} \sum_{i=1}^{n} \langle \boldsymbol{W}, \nabla_{\boldsymbol{W}} \ell(h_{\boldsymbol{W}}(\boldsymbol{x}_i), y_i) \rangle$	0.078
Path-norm [21]	$\sum_{(i_0,\dots,i_L)} \prod_{j=1}^{L} \left(\boldsymbol{W}_{i_j,i_{j-1}}\right)^2$	0.373

Table 1: Complexity measures compared in the empirical study [14], and their correlation with generalization

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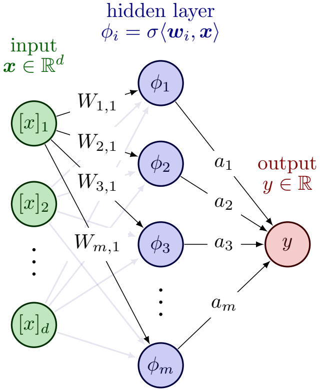
Two-layer neural networks, path norm

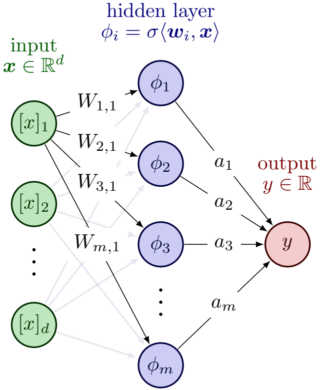


$$\mathcal{P}_m = \left\{ f_\theta(\cdot) := \frac{1}{m} \sum_{k=1}^m a_k \phi\big(\langle \boldsymbol{w}_k, \cdot\rangle\big) \right\}$$

ℓ_1-path norm

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

- semi-norm
- relations to Barron spaces $\mathcal{B}$ [2, 12]
  $\|f\|_{\mathcal{B}} \leq \|\boldsymbol{\theta}\|_{\mathcal{P}} \leq 2\|f\|_{\mathcal{B}}$



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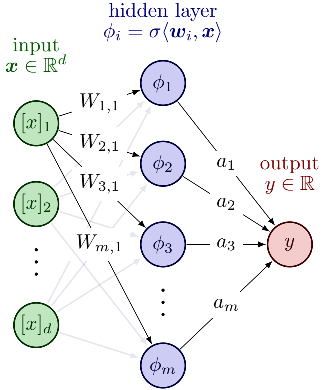

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*Path norm, Barron spaces, RKHS [11, 6]

Consider a random features model (RFM) [23, 17]

- first layer: $\boldsymbol{w} \overset{iid}{\sim} \mu \in \mathcal{P}(\mathcal{W})$; only train the second layer

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

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

- RFMs $\equiv$ kernel methods by taking $p = 2$ using Representer theorem [24]
- RFMs $\not\equiv$ kernel methods if $p < 2$
- function space: $\mathcal{F}_{\infty,\mu} \subseteq \mathcal{F}_{p,\mu} \subseteq \mathcal{F}_{q,\mu} \subseteq \mathcal{F}_{1,\mu}$ if $p \geq q$

For any $1 \leq p \leq \infty$, define

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- largest
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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

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

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Metric entropy: minimax?

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*

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

with some universal constant C *independent of* d.

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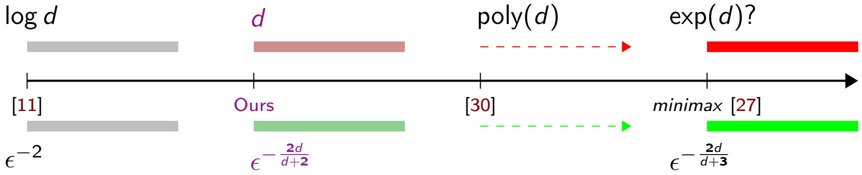
$$\log \mathcal{N}_2(\mathcal{G}_1, \epsilon) \leqslant C d \epsilon^{-\frac{2d}{d+2}}\,, \quad \forall \epsilon > 0 \quad \text{and} \quad d \geq 5\,,$$

with some universal constant C independent of d.



Metric entropy: minimax?

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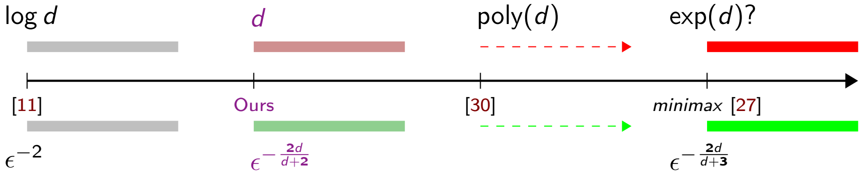

The “best” trade-off between ϵ and d.

Proof sketch: convex hull technique and its constant!

- Consider the following function space

$$\mathcal{F} = \{\sigma(\langle \widetilde{\boldsymbol{w}}, \cdot \rangle) : \widetilde{\boldsymbol{w}} \in \mathcal{W}\} \cup \{0\} \cup \{-\sigma(\langle \widetilde{\boldsymbol{w}}, \cdot \rangle) : \widetilde{\boldsymbol{w}} \in \mathbb{S}_1^{d-1} \text{ with the } \ell_1 \text{ ball}\}$$

- the convex hull of $\mathcal{F}$ is

$$\overline{\mathrm{conv}}\mathcal{F} = \left\{ \sum_{i=1}^m \alpha_i f_i \,\middle|\, f_i \in \mathcal{F}, \sum_{i=1}^m \alpha_i = 1, \alpha_i \geqslant 0, m \in \mathbb{N} \right\}.$$

- convex hull technique [29, Theorem 2.6.9]

$$\log \mathcal{N}_2(\mathcal{G}_1, \epsilon) \leqslant \log \mathcal{N}_2(\overline{\mathrm{conv}}\mathcal{F}, \epsilon, \mu) \leqslant C \left(\frac{1}{\epsilon}\right)^{\frac{2d}{d+2}}.$$

- control the constant C

$$C := \underbrace{D_k}_{=\Theta(d)} [\underbrace{C_k}_{=\Theta(1)} (2^{d+1}+1)^{\frac{1}{d}}]^{\frac{2d}{d+2}} \leq 10^7 d \quad \text{if } d > 5$$

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Optimization in Barron spaces is NP hard: curse of dimensionality! [1]

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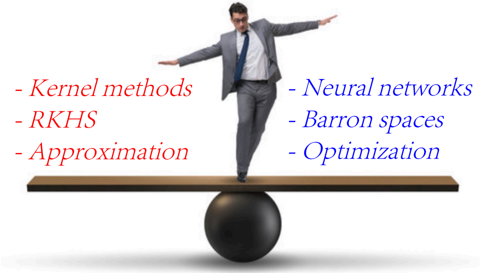

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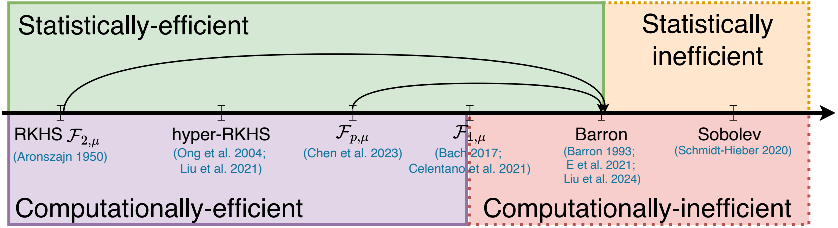

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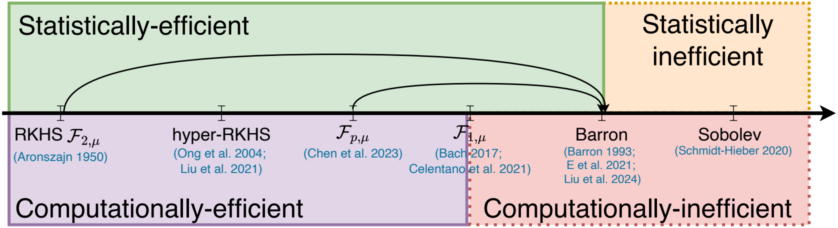

Do some Barron functions can be learned by two-layer NNs, both statistically and computationally efficient?

Learning with multiple ReLU neurons

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

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

$\|\hat{f} - f^\star\|_{L^2(\mathrm{d}\mu)} \leq \epsilon$ 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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How to do it by gradient descent

Learning multi ReLU neurons by two-layer NN via GD

$$L(\boldsymbol{W}) = \frac{1}{2}\mathbb{E}_{\boldsymbol{x}\sim\mathcal{N}(0,\boldsymbol{I}_d)}\left(\sum_{i=1}^{m}\sigma(\langle \boldsymbol{w}_i, \boldsymbol{x}\rangle) - f^\star(\boldsymbol{x})\right)^2$$

- Gaussian initialization for student neurons: $\boldsymbol{w}_i \sim \mathcal{N}(0, \sigma^2 \boldsymbol{I}_d)$
- angle: $\theta_{ij} \triangleq \angle(\boldsymbol{w}_i, \boldsymbol{v}_j)$, $\varphi_{ij} \triangleq \angle(\boldsymbol{w}_i, \boldsymbol{w}_j)$

Assumption

- *diverse teacher neurons: $\{\boldsymbol{v}_j\}_{j=1}^k$ are orthogonal and $\|\boldsymbol{v}_j\|_2 = \texttt{const}$*
- *warm start: the smallest angle not close to orthogonal*
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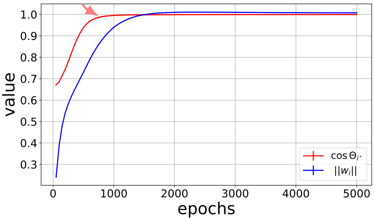
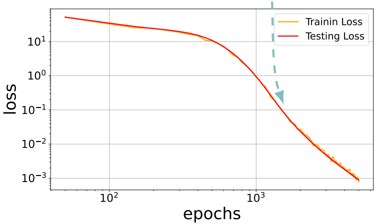
How does GD learn features and recover teacher neurons?

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





Theorem (Zhu, Liu, Cevher, 2024)

For sufficiently small initialization and step-size $\sigma, \eta = o(m^{-k^2})$, then after weak recovery, there exists a time $T_0 = \frac{1}{\eta}$ such that $\forall T \in \mathbb{N}$ and $i \in [m]$,

$$L(\mathbf{W}(T+T_0)) \le \mathcal{O}\left(\frac{1}{T^3}\right), \|\mathbf{w}_i(T+T_0)\|_2 = \Theta\left(\frac{k\|\mathbf{v}\|_2}{m}\right) \quad w.h.p.$$

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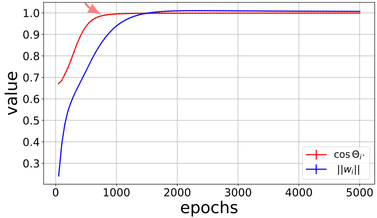

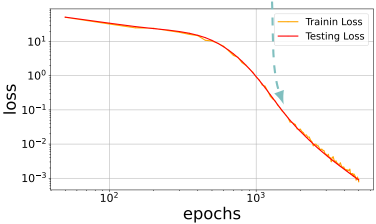

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Proof Sketch

- gradient expression $\nabla_i(t)$: a function of $\|\boldsymbol{w}_i\|, \|\boldsymbol{v}_i\|, \theta_{il}, \varphi_{ij}$
- Phase 1 (amplify alignment)
  - $\langle \boldsymbol{w}_i(t), \nabla_i(t)\rangle \leq 0 \Rightarrow \|\boldsymbol{w}_i(t)\|$ increasing
  - track $\theta_{i^\star}(t)$: linear convergence of $\sin\theta_{i^\star} \Rightarrow \theta_{i^\star}(t) \leq \epsilon_1$
- Phase 2 (norm convergence)
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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

- robust overfitting from the perspective of **approximation** [26]

well-separated data + target function is smooth enough + perturbation is small enough

$\Rightarrow$ **Avoid robust overfitting!**

- LoRA with low-rank dynamics: from **statistical** to **computational**

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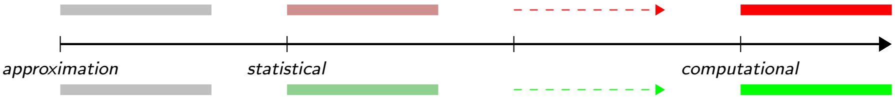

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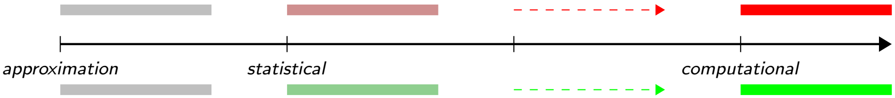

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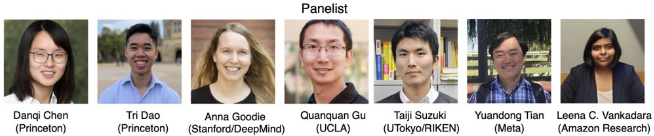
We're organizing Fine-tuning workshop at NeurIPS 2024!

Fine-Tuning in Modern Machine Learning: Principles and Scalability

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



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*Separation between robust and clean generalization

	#parameters	Upper bound
standard generalization	$\mathcal{O}(nd)$	$\widetilde{\mathcal{O}}\left(n^{-\frac{2\alpha}{2\alpha+d}}\right)$
robust generalization	$\mathcal{O}\left(nd + \delta^{-\frac{d}{2\alpha-2}} \log \frac{1}{\delta}\right)$	$\mathcal{O}(\sqrt{d}\delta)$

- more smooth, less #params
- Examples: $\delta < n^{-\frac{1}{d-1}}$
  - $\delta = \frac{1}{n}$: robust overfitting?

well-separated data + target function is smooth enough + perturbation is small enough

$\Rightarrow$ **Avoid robust overfitting!**

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