The Role of Over-parameterization in Statistical Machine Learning

- a function space perspective

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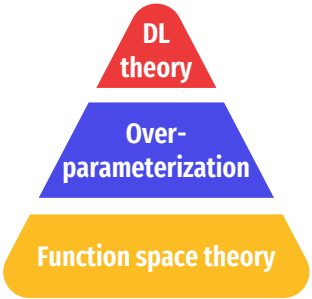
Today's Over-parameterization journey - *the good, the bad, the ugly*

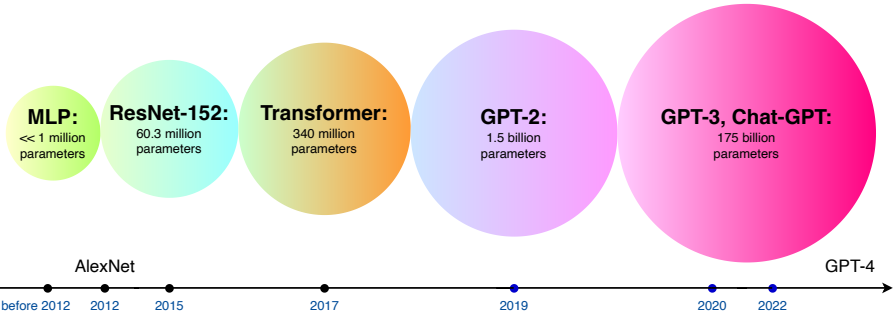


Helps robustness or not?

Why generalize well?

Motivation

Over-parameterization: more parameters than training data



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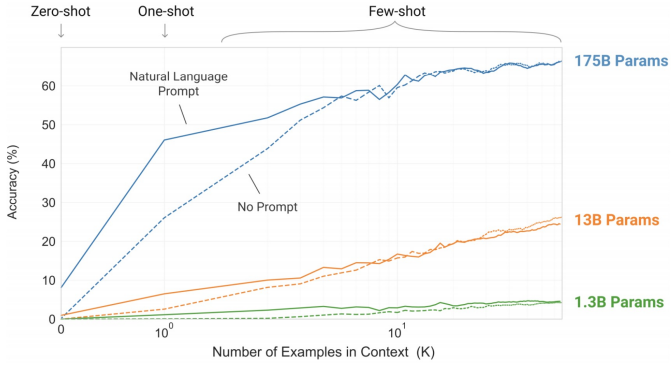

Figure: Larger models make increasingly efficient use of in-context information: source from Open AI.

DNNs: the good in fitting ...

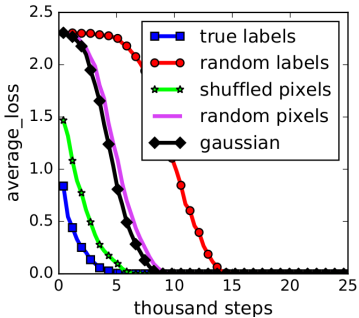

Figure: DNN Training curves on CIFAR10, from [1]

- A gap between theory and practice:
  - DNNs can fit random labels
  - SGD: zero training error and low test error

DNNs: the bad in robustness...

(a) Invisibility [2]

(b) Stop sign classified as 45 mph sign [3]

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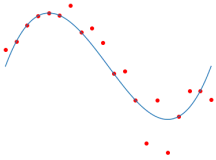
the ugly in over-parameterization?

A toy example: curve fitting



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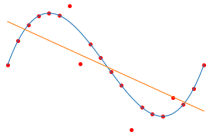

(a) under-fitting

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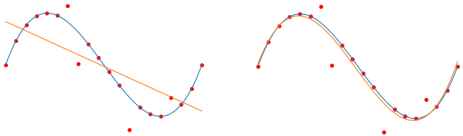

(a) under-fitting (b) sweet spot

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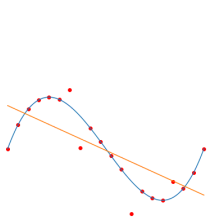

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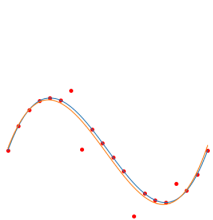

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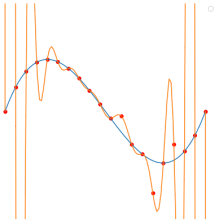

(c) overfitting

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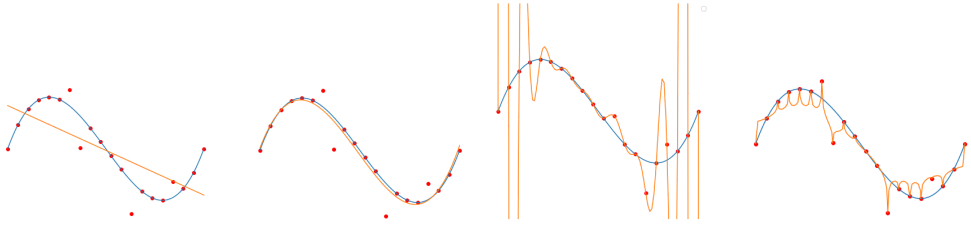

(a) under-fitting (b) sweet spot (c) overfitting (d) benign overfitting [4]

Figure: Test performance on curve fitting: source from Open AI.

Benign overfitting and double descent

benign overfitting [4, 5, 6]:

- model is very complex
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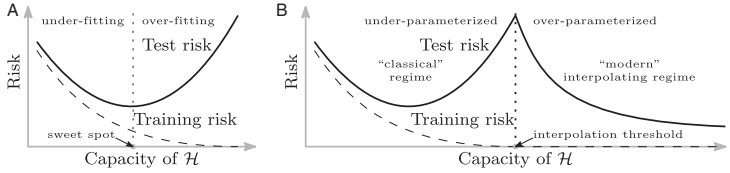
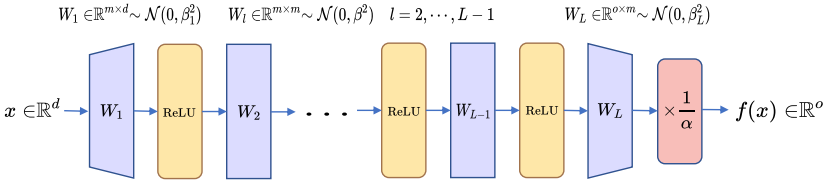


Figure: classical learning theory vs. double descent: source from [7].

Typical architecture of DNNs



Initialization	Formulation
LeCun initialization	$\beta_1 = \sqrt{\frac{1}{d}}$, $\beta = \beta_L = \sqrt{\frac{1}{m}}$
He initialization	$\beta_1 = \sqrt{\frac{2}{d}}$, $\beta = \beta_L = \sqrt{\frac{2}{m}}$
NTK initialization	$\beta = \beta_1 = \sqrt{\frac{2}{m}}$, $\beta_L = 1$
Xavier initialization	$\beta_1 = \frac{2}{m+d}$, $\beta = \frac{1}{m}$, $\beta_L = \frac{2}{m+1}$

Why function space theory is needed? (lazy training regime)

$$\mathcal{F}_{\mathrm{NN},m} = \left\{ f_m(\boldsymbol{x};\boldsymbol{\Theta}) = \sum_{i=1}^{m} a_i \max\left(\langle \boldsymbol{w}_i, \boldsymbol{x}\rangle, 0\right) : a_i \in \mathbb{R}, \boldsymbol{w}_i \in \mathbb{R}^d \right\}$$

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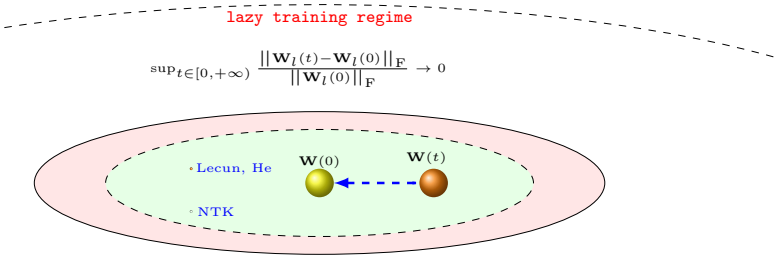

Figure: Training dynamics of two-layer ReLU NNs under different initializations [8, 9, 10].

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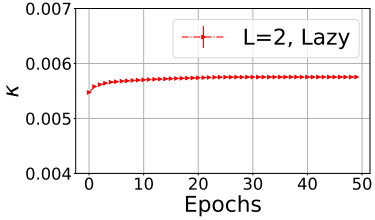
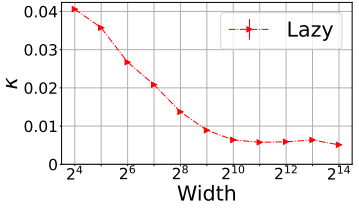
$$\text{lazy training ratio } \kappa := \frac{\sum_{l=1}^{L} \|\boldsymbol{W}_l(t) - \boldsymbol{W}_l(0)\|_{\mathrm{F}}}{\sum_{l=1}^{L} \|\boldsymbol{W}_l(0)\|_{\mathrm{F}}}$$





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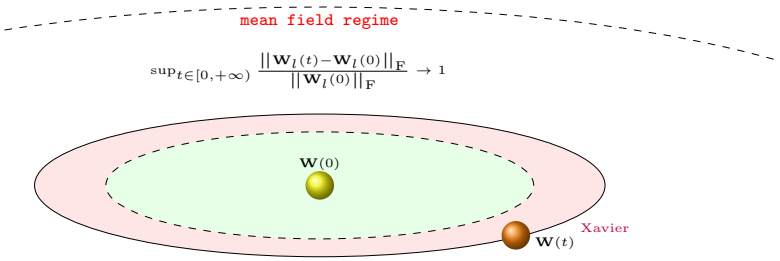

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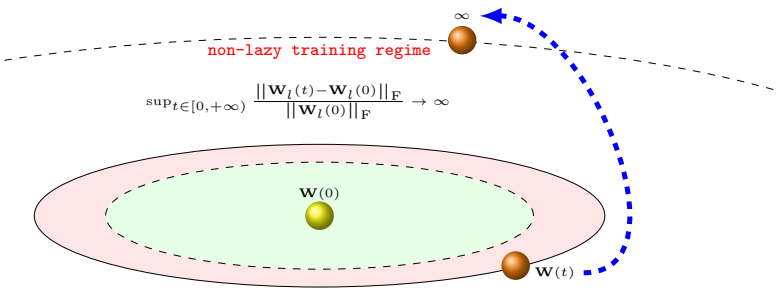

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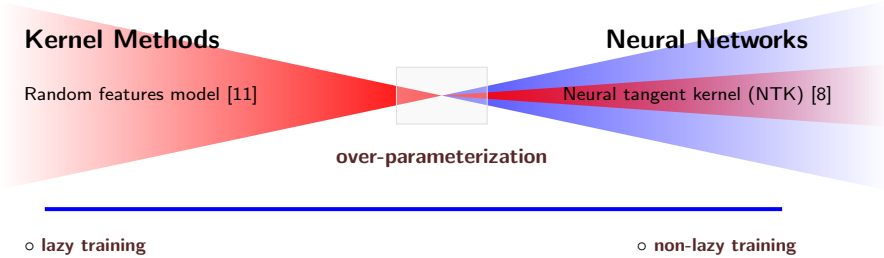
Research Overview: Today's talk



- **generalization** of NNs
  - [LSC, NeurIPS22] why **over-parameterized NNs** generalize well under SGD training?
- **robustness** of NNs
  - [ZLCC, NeurIPS22] **Over-parameterization** helps or hurts robustness of NNs?

Obstacle in modern ML setting

Modern ML setting

comparably large: #training data n, #parameters m, input dimension d

- high dimensional setting [12, 13]: $c \leqslant \{d/n, m/n\} \leqslant C$

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$$\text{ridge regression: } \hat{\boldsymbol{\beta}} = (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I})^{-1} \boldsymbol{X}^\top \boldsymbol{y} \xrightarrow{?} \boldsymbol{\beta}^\star := \arg\min_{\boldsymbol{\beta}} \mathbb{E}[(\boldsymbol{y} - \boldsymbol{\beta}^\top \boldsymbol{x})^2]$$

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Consistency of estimator?

- classical low-dimensional setting (d fixed and $n \to \infty$): ✓
- classical high-dimensional setting ($d \gg n$) if sparsity [14]: ✓
- n, d, m are comparably large: ✗

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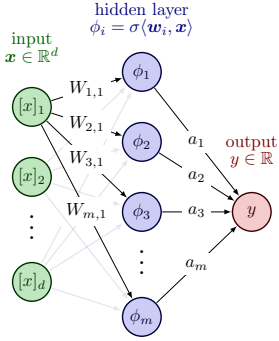
for what sample size, and what data distributions, the estimator can generalize well?

Problem settings



random features mapping [11]:

$$\varphi(\boldsymbol{x}) := \frac{1}{\sqrt{m}}\sigma\left(\frac{\boldsymbol{W}\boldsymbol{x}}{\sqrt{d}}\right), \quad W_{ij} \sim \mathcal{N}(0,1)$$

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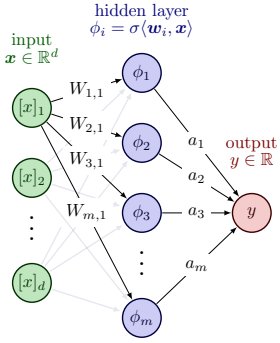

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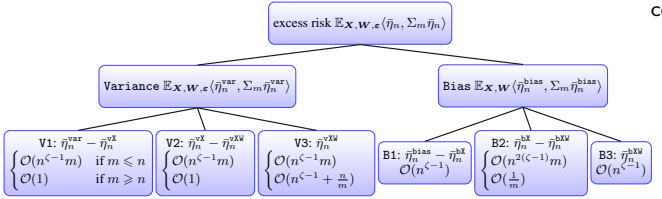
adaptive step-size SGD with one-pass iterate-averaging

$$\boldsymbol{a}_t = \boldsymbol{a}_{t-1} + \gamma_t[y_t - \langle \boldsymbol{a}_{t-1}, \varphi(\boldsymbol{x}_t)\rangle]\varphi(\boldsymbol{x}_t), \qquad t = 1, 2, \dots n\,.$$

- adaptive step-size: $\gamma_t := \gamma_0 t^{-\zeta}, \zeta \in [0, 1)$
- iterate-averaging: $\bar{\boldsymbol{a}}_n := \frac{1}{n}\sum_{t=0}^{n-1} \boldsymbol{a}_t$

Results: Bias and variance decomposition

Theorem [LSC, NeurIPS22]: Under sub-Gaussian data, label noise with bounded variance, we have



covariance operator: fast decay

- covariance operator: $\Sigma_m := \mathbb{E}_{\boldsymbol{x}}[\varphi(\boldsymbol{x}) \otimes \varphi(\boldsymbol{x})]$ (r.v.)
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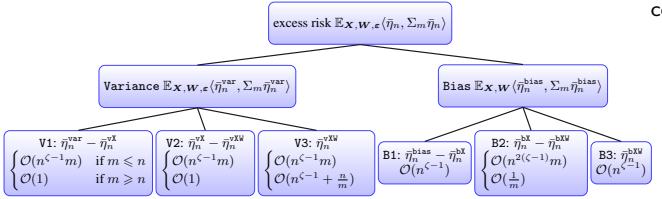

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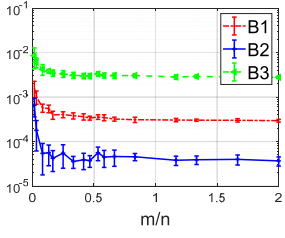
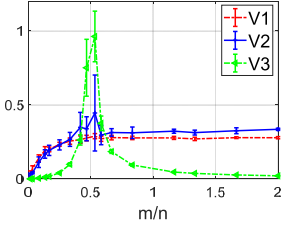
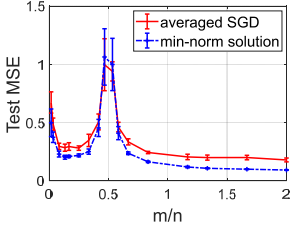


(a) Bias $\lesssim$ B1 + B2 + B3

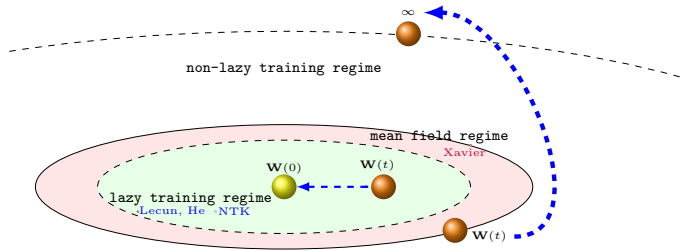


(b) Variance $\lesssim$ V1 + V2 + V3



(c) excess risk

From kernel methods to neural networks



kernel methods

- high dimensional kernel methods: only learn linear function! [12]
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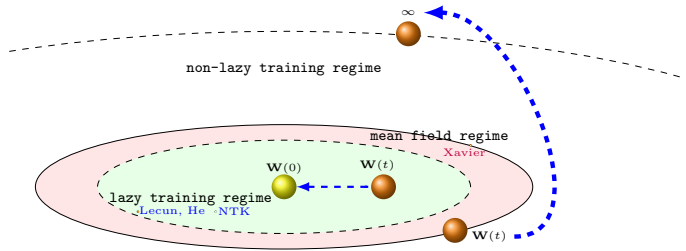

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Follow-up:

- function space: function space for neural networks, e.g., Barron space [15, 16]
- benign overfitting: Benign overfitting in deep neural networks under lazy training [ZLCLC, ICML23]

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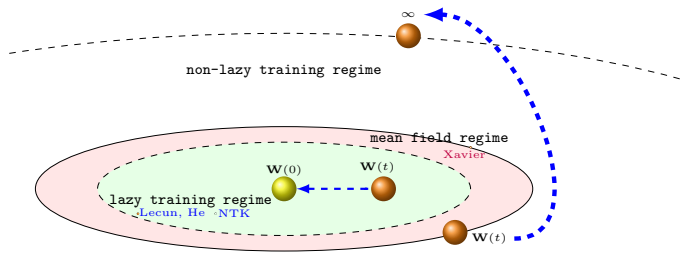

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- benign overfitting: Benign overfitting in deep neural networks under lazy training [ZLCLC, ICML23]
- Benign overfitting leads to huge sensitivity! [4]

Over-parameterization helps or hurts robustness?

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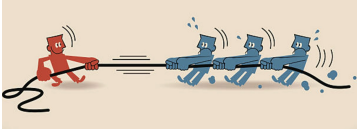

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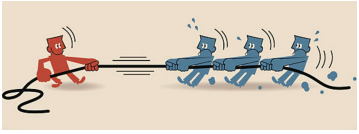

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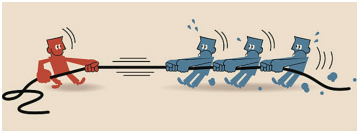

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The perturbation stability of a ReLU DNN $f(\boldsymbol{x}; \boldsymbol{W})$ is

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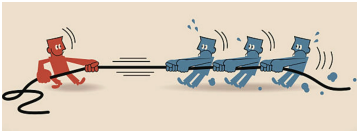

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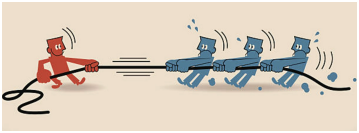

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where ϵ is the perturbation radius.

Main results (Lazy-training regime)

Theorem[ZLCC, NeurIPS22]: $\cdot \lesssim \mathrm{Func}(m, L, \beta)$

Assumption	Initialization	Our bound for $\mathscr{P}(f,\epsilon)/\epsilon$	Trend of width m [1]	Trend of depth L [1]
$\|\boldsymbol{x}\|_2 = 1$	LeCun initialization	$\left(\sqrt{\frac{L^3 m}{d}} e^{-m/L^3} + \sqrt{\frac{1}{d}}\right)(\frac{\sqrt{2}}{2})^{L-2}$	↗ ↘	↘
	He initialization	$\sqrt{\frac{L^3 m}{d}} e^{-m/L^3} + \sqrt{\frac{1}{d}}$	↗ ↘	↗
	NTK initialization	$\sqrt{\frac{L^3 m}{d}} e^{-m/L^3} + 1$	↗ ↘	↗

[1] The larger perturbation stability means worse average robustness.

Takeaway messages: **the good (width), the bad (depth), the ugly (initialization)**

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Theorem[ZLCC, NeurIPS22]: $\cdot \lesssim \mathrm{Func}(m, L, \beta)$

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	He initialization	$\sqrt{\frac{L^3 m}{d}} e^{-m/L^3} + \sqrt{\frac{1}{d}}$	↗ ↘	↗
	NTK initialization	$\sqrt{\frac{L^3 m}{d}} e^{-m/L^3} + 1$	↗ ↘	↗

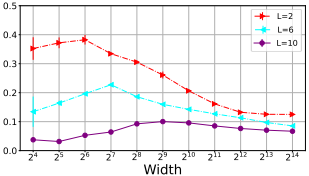
[1] The larger perturbation stability means worse average robustness.

Takeaway messages: **the good (width), the bad (depth), the ugly (initialization)**

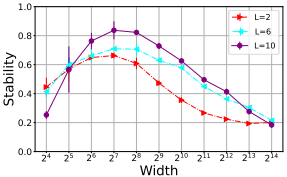
- width **helps** robustness in the over-parameterized regime
- depth **helps** robustness in LeCun initialization but **hurts** robustness in He/NTK initialization

Experiments: robustness under lazy-training regime

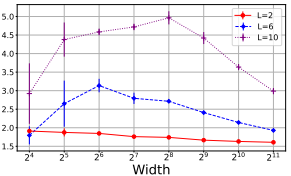
Metrics	Ours (NTK initialization)	[19]	[20]
$\mathscr{P}(f,\epsilon)/\epsilon$	$\sqrt{\frac{L^3 m}{d}} e^{-m/L^3} + 1$	$L^2 m^{1/3} \sqrt{\log m} + \sqrt{mL}$	$2^{\frac{3L-5}{2}} \sqrt{L}$



(a) LeCun initialization



(b) He initialization



(c) NTK initialization

Proof sketch in robustness

$$
\begin{aligned}
\mathscr{P}(\boldsymbol{f}, \epsilon) &:= \mathbb{E}_{\boldsymbol{x},\hat{\boldsymbol{x}},\boldsymbol{W}} \left\|\nabla_{\boldsymbol{x}} \boldsymbol{f}(\boldsymbol{x})(\boldsymbol{x}-\hat{\boldsymbol{x}})\right\|_2 \\
&\leq \mathbb{E}_{\boldsymbol{x},\hat{\boldsymbol{x}},\boldsymbol{W}} \left\|\nabla_{\boldsymbol{x}} \boldsymbol{f}(\boldsymbol{x})(\boldsymbol{x}-\hat{\boldsymbol{x}}) - \boldsymbol{W}_L \boldsymbol{D}_{L-1} \boldsymbol{W}_{L-1} \cdots \boldsymbol{D}_1 \boldsymbol{W}_1 (\boldsymbol{x}-\hat{\boldsymbol{x}})\right\|_2 + \mathbb{E}_{\boldsymbol{x},\hat{\boldsymbol{x}},\boldsymbol{W}} \left\|\boldsymbol{W}_L \boldsymbol{D}_{L-1} \boldsymbol{W}_{L-1} \cdots \boldsymbol{D}_1 \boldsymbol{W}_1 (\boldsymbol{x}-\hat{\boldsymbol{x}})\right\|_2 \\
&\leq \mathbb{E}_{\boldsymbol{x},\hat{\boldsymbol{x}},\boldsymbol{W}} \left\|[\nabla_{\boldsymbol{x}} \boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{W}_L \boldsymbol{D}_{L-1} \boldsymbol{W}_{L-1} \cdots \boldsymbol{D}_1 \boldsymbol{W}_1](\boldsymbol{x}-\hat{\boldsymbol{x}})\right\|_2 + \sqrt{\mathbb{E}_{\boldsymbol{x},\hat{\boldsymbol{x}},\boldsymbol{W}} \left\|\boldsymbol{W}_L \underbrace{\boldsymbol{D}_{L-1} \boldsymbol{W}_{L-1} \cdots \boldsymbol{D}_1 \boldsymbol{W}_1 (\boldsymbol{x}-\hat{\boldsymbol{x}})}_{:=\boldsymbol{t}_L}\right\|_2^2} \\
&\lesssim \epsilon \left(\sqrt{L^3 m^2 \beta_1^2 \beta_L^2} e^{-m/L^3} + \sqrt{mo \beta_1^2 \beta_L^2} \right) \gamma^{L-2},
\end{aligned}
$$

where we use $\mathbb{E}_{\boldsymbol{W}} \frac{\|\boldsymbol{t}_l\|_2^2}{\left\|\boldsymbol{t}_{l-1}\right\|_2^2} = \gamma^2$ with $\gamma := \beta / \sqrt{\frac{2}{m}}$.

Main results (Non-lazy training regime)

A sufficient condition for DNNs

For large enough m and $m \gg d$, w.h.p, DNNs fall into non-lazy training regime if $\alpha \gg (m^{3/2} \sum_{i=1}^{L} \beta_i)^L$.

Remarks: $\circ$ $L = 2$, $\alpha = 1$, $\beta_1 = \beta_2 = \beta \sim \frac{1}{m^c}$ with $c > 1.5$

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Theorem (non-lazy training regime for two-layer NNs)

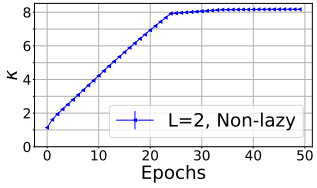
Under this setting with $m \gg n^2$ and standard assumptions, then

$$\textit{perturbation stability} \leq \widetilde{\mathcal{O}}\left(\frac{n}{m^{c+1.5}}\right), \ w.h.p$$

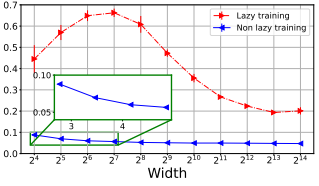
Remarks: ○ width helps robustness in the over-parameterized regime in both lazy/non-lazy training regime

Experiment: Non-lazy training regime

$$\text{lazy training ratio } \kappa := \frac{\sum_{l=1}^{L} \|\boldsymbol{W}_l(t) - \boldsymbol{W}_l(0)\|_{\mathrm{F}}}{\sum_{l=1}^{L} \|\boldsymbol{W}_l(0)\|_{\mathrm{F}}}$$



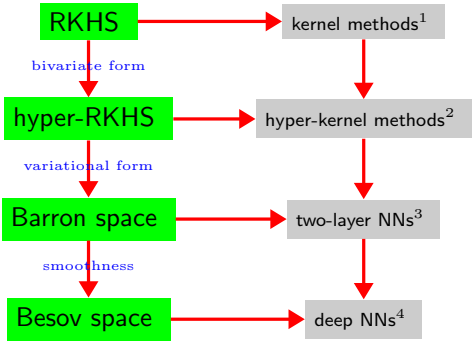
(a) lazy training ratio *vs.* epochs

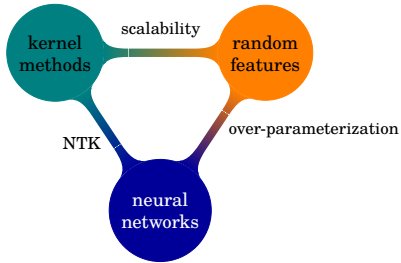


(b) perturbation stability

Conclusion(I) function spaces vs. models

Understanding from a function space perspective!





[1] [LHGYL, JMLR20; LHCS, TPAMI21; LLS, AISTATS21]

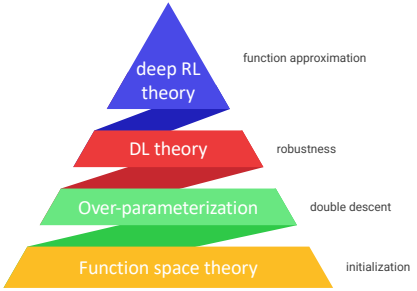
[2] [LSHYS, JMLR21]

[3] [LSC, NeurIPS22; LHCS, TPAMI22; LHCS, AISTATS21]

[4] [LVC, NeurIPS22; ZLCC, NeurIPS22; WZLCC, NeurIPS22, ZLCLC, ICML23]

Conclusion(II) the good, the bad, the ugly

	good	bad	ugly
kernel methods	analysis	performance	curse of dimensionality
neural networks	performance	analysis	over-parameterization
generalization	benign overfitting	catastrophic overfitting	model complexity
robustness	width	depth	initialization



- IEEE ICASSP 2023 Tutorial - "Neural networks: the good, the bad, and the ugly"
- CVPR 2023 Tutorial - "Deep learning theory for computer vision"

Thanks for your attention!

Q & A

my homepage www.lfhsgre.org for more information!

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