Disentangling Trainability and Generalization in Deep Neural Networks

Lechao Xiao, Jeffrey Pennington, Samuel Schoenholz

Notation

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- Fully-connected L-layer network:

$$\boldsymbol{z}^{(l+1)}(\boldsymbol{x}) = \frac{\sigma_w}{\sqrt{d_l}} \boldsymbol{W}^{(l+1)} \phi\left(\boldsymbol{z}^{(l)}(\boldsymbol{x})\right) + \sigma_b \boldsymbol{b}^{(l+1)}$$

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- We can control **variances** σ_w, σ_b and study how the network behaves when varying these

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- Stack features and targets into matrices:

$$\boldsymbol{X} \in \mathbb{R}^{n \times d_0} \text{ and } \boldsymbol{y} \in \mathbb{R}^{n}$$

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1) $\Sigma^{(1)}(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{x}^T \boldsymbol{x}'$

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- If network has **multiple** outputs:

$$f_{\boldsymbol{\theta},i} \perp f_{\boldsymbol{\theta},j}$$

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- **Infinite-width** limit:

Deterministic and time-independent

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$$\begin{aligned} f_\infty(\boldsymbol{x}) &= \left(\mathbf{\Theta}^{(L)}(\boldsymbol{x}, \boldsymbol{X})\right)^T \left(\mathbf{\Theta}^{(L)}(\boldsymbol{X}, \boldsymbol{X})\right)^{-1} \boldsymbol{y} \\ &= P(\mathbf{\Theta}^{(L)})\boldsymbol{y} \end{aligned}$$

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- We are assuming $f_0(\boldsymbol{x}) = 0$ here

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- What happens if we let **depth** L go to infinity as well?

Large-Depth Limit

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Two kinds of limits:

- Take width and depth to infinity **simultaneously**
- Take width limit **first** and **then** consider depth limit
- Two **different** results!

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$\implies$ **Feature-learning** happening!

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- Consider the **sequential limit**
- **Incremental**:
  - "*Exponential expressivity in deep neural networks through transient chaos*"
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- Connect **chaotic** and **ordered** regimes with generalization and trainability
- How to characterize **generalization** and **trainability**?

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- Recall that we have closed-form training dynamics:

$$f_t(\boldsymbol{x}) = \boldsymbol{\Theta}^{(L)}(\boldsymbol{x}, \boldsymbol{X}) \left(\boldsymbol{\Theta}^{(L)}(\boldsymbol{X}, \boldsymbol{X})\right)^{-1} \left(\mathbb{1} - e^{-t\eta \boldsymbol{\Theta}^{(L)}(\boldsymbol{X}, \boldsymbol{X})}\right) \boldsymbol{y}$$

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- **Diagonalize** NTK: $\boldsymbol{\Theta}^{(L)}(\boldsymbol{X}, \boldsymbol{X}) = \boldsymbol{U}^T \boldsymbol{\Lambda} \boldsymbol{U}$ which leads to

rotated labels

$$\tilde{f}_{t,i}(\boldsymbol{X}) = \left(\mathbb{1} - e^{-t\eta\lambda_i}\right) \tilde{y}_i$$

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$\implies$ **Cannot** learn training set

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- Different regimes (chaotic and ordered) in the (σ_w, σ_b) plane where $P(\boldsymbol{\Theta}^{(\infty)})$ is **data-dependent** or **data-independent**
- Data-dependence of course **not** best measure to study generalization performance

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- Study trajectory of $P(\mathbf{\Theta}^{(l)})$ to understand generalization

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- **Attracting** or **repulsive** fixed point?

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$$f(c) = \frac{1}{q^*}\left(\sigma_w^2 \int \phi\left(u_1(z_1)\right)\phi\left(u_2(z_1, z_2, c)\right)\mathcal{D}z_1\mathcal{D}z_2 + \sigma_b^2\right)$$

- **Observe:** $f(1) = 1 \implies c^* = 1$ is a fixed point of f

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- Turns out: $f'(1) = \sigma_w^2 \int \left[\phi'(\sqrt{q^*}z)\right]^2 \mathcal{D}z$

  $\implies$ Depends on σ_w and σ_b

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  Two outputs thus become more and more **dissimilar** to each other

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$= \mathbb{E}_{z \sim \mathcal{N}\left(0, \begin{pmatrix} q^* & q_{ab}^{(l)} \\ q_{ab}^{(l)} & q^* \end{pmatrix}\right)} \left[\phi(z_1)\phi(z_2)\right]$

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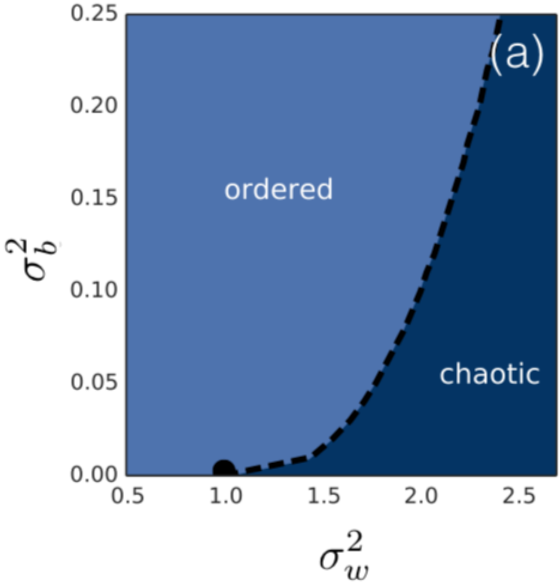
- Analyze the limits in the two different regimes

An Example



0.25
0.20
0.15
0.10
0.05
0.00
0.5
1.0
1.5
2.0
2.5
(a)
ordered
chaotic
σ_b^2
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$\implies$ Networks become **untrainable**!

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- Define $\epsilon_{ab}^{(l)} = q_{ab}^{(l)} - q_{ab}^{*}$ and $\delta_{ab}^{(l)} = p_{ab}^{(l)} - p_{ab}^{*}$
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- **Hence:** $\epsilon_{ab}^{(l+1)} \approx \sigma_w^2 \dot{\mathcal{T}}\left(q_{ab}^{*}\right) \epsilon_{ab}^{(l)} = f'(c^*)^{l+1} \epsilon_{ab}^{(0)}$
- **Similarly:** $\delta_{ab}^{(l+1)} \approx f'(c^*)^{l+1} \left(\delta_{ab}^{(0)} + l\left(1 + \frac{f''(c^*)}{f'(c^*)} p_{ab}^{*}\right) \epsilon_{ab}^{(0)}\right)$

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- We hence get the trivial prediction **independent** of the data!

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  $\implies$ Network **fails** to generalize

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- More **subtle**: Can't use continuity of map

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- width correction matrix that depends on the data
- $A^{(l)}(X,X) \longrightarrow A^{(\infty)}(X,X$

- Write $\boldsymbol{\Theta}^{(l)}(\boldsymbol{X}, \boldsymbol{X}) = p^* \mathbf{1}\mathbf{1}^T + l\,(f'(1))^l\,\boldsymbol{A}^{(l)}(\boldsymbol{X}, \boldsymbol{X})$

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$$= \lambda^{-1}\left(\left(\boldsymbol{A}_{\boldsymbol{X}}^{(j)}\right)^{-1} - \hat{p}\boldsymbol{a}\boldsymbol{a}^T\right)$$

$a = (A_X^{(j)})^{-1}\underline{1}$

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  Non-trivial generalization possible!

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- $\lim_{l \to \infty} \kappa \left(\boldsymbol{\Theta}^{(l)}(\boldsymbol{X}, \boldsymbol{X})\right) = \infty \implies$ Becomes **untrainable**

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- $\lim_{l \to \infty} \lambda_1 \left(\mathbf{\Theta}^{(l)}(\boldsymbol{X}, \boldsymbol{X})\right) = np^*$
- $\lim_{l \to \infty} \lambda_{\text{bulk}} \left(\mathbf{\Theta}^{(l)}(\boldsymbol{X}, \boldsymbol{X})\right) = 0$
- $\lim_{l \to \infty} \kappa \left(\mathbf{\Theta}^{(l)}(\boldsymbol{X}, \boldsymbol{X})\right) = \infty \implies$ Becomes **untrainable**
- $\lim_{l \to \infty} f_{\infty}^{(l)}(\boldsymbol{x}) = \left(\boldsymbol{A}_{\boldsymbol{z}}^{(\infty)} \left(\boldsymbol{A}_{\boldsymbol{X}}^{(\infty)}\right)^{-1} + \hat{\boldsymbol{A}}\right) \boldsymbol{y}$

Ordered Regime: Summary

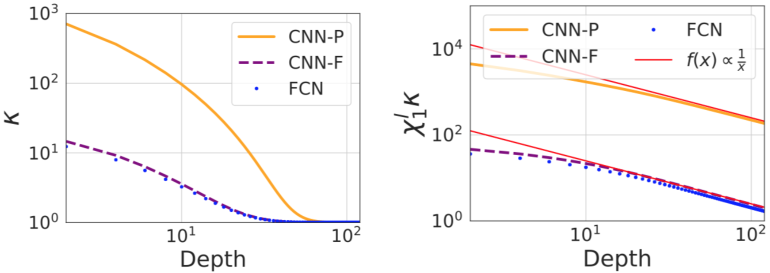
- Characterized by $f'(1) = \sigma_w^2 \int \left[\phi'(\sqrt{q^*}z)\right]^2 \mathcal{D}z < 1$
- $\lim_{l \to \infty} \lambda_1 \left(\boldsymbol{\Theta}^{(l)}(\boldsymbol{X}, \boldsymbol{X})\right) = np^*$
- $\lim_{l \to \infty} \lambda_{\text{bulk}} \left(\boldsymbol{\Theta}^{(l)}(\boldsymbol{X}, \boldsymbol{X})\right) = 0$
- $\lim_{l \to \infty} \kappa \left(\boldsymbol{\Theta}^{(l)}(\boldsymbol{X}, \boldsymbol{X})\right) = \infty \implies$ Becomes **untrainable**
- $\lim_{l \to \infty} f_\infty^{(l)}(\boldsymbol{x}) = \left(\boldsymbol{A}_{\boldsymbol{z}}^{(\infty)} \left(\boldsymbol{A}_{\boldsymbol{X}}^{(\infty)}\right)^{-1} + \hat{\boldsymbol{A}}\right) \boldsymbol{y}$

  $\implies$ Network might be **able** to generalize

Experiments (I)

Chaotic: $\kappa \to 1$

ordered: $\kappa \simeq (\chi_1^l \cdot c)^{-1} \to \infty$

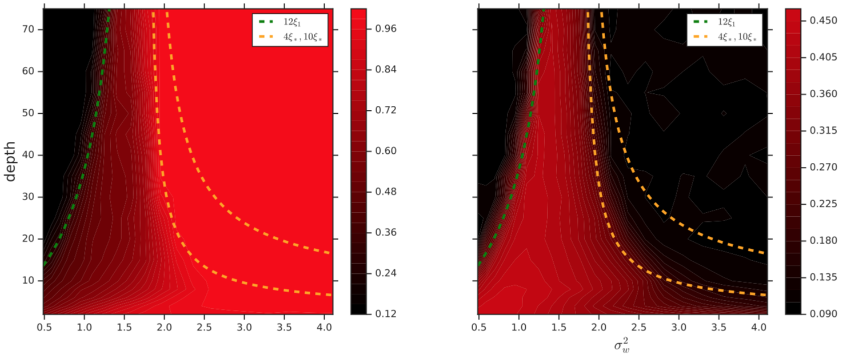


Condition number in the chaotic and ordered regime

Experiments (II)

Train accuracy

Test accuracy



Test and Training Accuracy for Finite Depth and Width Networks

Discussion

- Important to also study **infinite depth**, after all seems to be more important in practice than big widths
- Interesting **tradeoff** between generalization and trainability
- Characterization of generalization a bit **weak** but seems to be true empirically
- Approximation of the diagonal $\Sigma^{(l)}(\boldsymbol{x}, \boldsymbol{x}) = q^*$ **very strong** assumption, unclear how this affects the obtained limits
- Very **messy** paper, lots of referencing to prior work and some statements are a bit unclear