Generalization of Deep ResNets in the Mean-Field Regime

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OverView

Question:

- Can we build a generalization analysis of trained Deep ResNets in the mean-field setting?

Contributions:

- The first **minimum eigenvalue estimation** (lower bound) of the Gram matrix of the gradients for deep ResNet parameterized by the ResNet encoder's parameters and MLP predictor's parameters in the mean-field regime.
- The paper proves that the **KL divergence** of feature encoder ν and output layer ν can be bounded by a constant (depending only on network architecture parameters) during the training, which facilitates our generalization analysis.
- This paper builds the connection between the Rademacher complexity result and KL divergence, and then derive the **convergence rate** $\mathcal{O}(1/\sqrt{n})$ **for generalization**.

Problem Settings

Basic Settings:

- The training set $\mathcal{D}_n = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ is drawn from an unknown distribution μ on $\mathcal{X} \times \mathcal{Y}$, and μ_X is the marginal distribution of μ over $\mathcal{X}$.
- We consider a binary classification task, denoted by minimizing the expected risk, let $\ell_{0-1}(f, y) := \mathbb{1}\{yf < 0\}$.
- We employ the squared loss in ERM in training, i.e, $\ell(f, y) := \frac{1}{2}(y - f)^2$.
- The hypothesis f is parameterized by the ResNet feature encoder and a non-linear predictor, $f_{\tau,\nu}$. The empirical loss $\widehat{L}(\tau, \nu) := \mathbb{E}_{\boldsymbol{x} \sim \mathcal{D}_n} \, \ell(f_{\tau,\nu}(\boldsymbol{x}), y(\boldsymbol{x}))$.

Problem Settings

Network Structure: (α, β will be determined later)

- Discrete

$$\begin{aligned} \boldsymbol{z}_{l+1}(\boldsymbol{x}) &= \boldsymbol{z}_l(\boldsymbol{x}) + \frac{\alpha}{ML} \sum_{m=1}^{M} \boldsymbol{\sigma}(\boldsymbol{z}_l(\boldsymbol{x}), \boldsymbol{\theta}_{l,m}) \in \mathbb{R}^d, \quad l \in [L-1], \\ f_{\boldsymbol{\Omega}_K, \boldsymbol{\Theta}_{L,M}}(\boldsymbol{x}) &= \frac{\beta}{K} \sum_{k=1}^{K} h(\boldsymbol{z}_L, \boldsymbol{\omega}_k) \in \mathbb{R}, \end{aligned} \tag{1}$$

- The following ODE models the infinite death infinite width ResNet.

$$\frac{\mathrm{d}\boldsymbol{z}(\boldsymbol{x}, s)}{\mathrm{d}s} = \alpha \cdot \int_{\mathbb{R}^{k_\nu}} \boldsymbol{\sigma}(\boldsymbol{z}(\boldsymbol{x}, s), \boldsymbol{\theta}) \mathrm{d}\nu(\boldsymbol{\theta}, s), \ \ s \in [0,1], \ \ \boldsymbol{z}(\boldsymbol{x}, 0) = \boldsymbol{x}\,. \tag{2}$$

  We denote the solution of Equation (2) as $\boldsymbol{Z}_\nu(\boldsymbol{x}, s)$.

- The whole network can be written as

$$f_{\tau,\nu}(\boldsymbol{x}) := \beta \cdot \int_{\mathbb{R}^{k_\tau}} h(\boldsymbol{Z}_\nu(\boldsymbol{x}, 1), \boldsymbol{\omega}) \mathrm{d}\tau(\boldsymbol{\omega}),$$

Assumptions

Assumption (Assumptions on data)

We assume that for $\boldsymbol{x}_i \neq \boldsymbol{x}_j \sim \mu_X$*, the following holds with probability 1,*

$$\|\boldsymbol{x}_i\|_2 = 1, |y(\boldsymbol{x}_i)| \leq 1, \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle \leq C_{\max} < 1\,, \forall i, j \in [n]\,.$$

Assumption (Assumption on initialization)

The initial distribution τ_0, ν_0 *is standard Gaussian:* $(\tau_0, \nu_0)(\boldsymbol{\omega}, \boldsymbol{\theta}, s) \propto \exp\left(-\frac{\|\boldsymbol{\omega}\|_2^2 + \|\boldsymbol{\theta}\|_2^2}{2}\right), \forall s \in [0, 1]$.

Assumptions (continued)

Assumption (Assumptions on activation $\boldsymbol{\sigma}, h$)

Let $\boldsymbol{\theta} := (\boldsymbol{u}, \boldsymbol{w}, b) \in \mathbb{R}^{k_\nu}$*, where* $\boldsymbol{u}, \boldsymbol{w} \in \mathbb{R}^{k_\nu}, b \in \mathbb{R}$*, i.e.* $k_\nu = 2d + 1$*;* $\boldsymbol{\omega} := (a, \boldsymbol{w}, b) \in \mathbb{R}^{k_\tau}$*, where* $\boldsymbol{w} \in \mathbb{R}^{k_\nu}, a, b \in \mathbb{R}$*, i.e.* $k_\tau = d + 2$*. For any* $\boldsymbol{z} \in \mathbb{R}^{k_\nu}$*, we assume*

$$\boldsymbol{\sigma}(\boldsymbol{z}, \boldsymbol{\theta}) = \boldsymbol{u}\sigma_0(\boldsymbol{w}^\top \boldsymbol{z} + b), \quad h(\boldsymbol{z}, \boldsymbol{\omega}) = a\sigma_0(\boldsymbol{w}^\top \boldsymbol{z} + b), \quad \sigma_0 : \mathbb{R} \to \mathbb{R}.$$

In addition, we have the following assumption on σ_0*.* $|\sigma_0(x)| \leq C_1 \max(|x|, 1), |\sigma_0'(x)| \leq C_1, |\sigma_0''(x)| \leq C_1$*, and let* $\mu_i(\sigma_0)$ *be the* i*-th Hermite coefficient of* σ_0*.*

Gradient Evolution

- The evolution of the ResNet layers $\nu(\boldsymbol{\theta}, s)$ can be characterized as

$$\frac{\partial \nu}{\partial t}(\boldsymbol{\theta}, s, t) = \nabla_{\boldsymbol{\theta}} \cdot \left(\nu(\boldsymbol{\theta}, s, t) \nabla_{\boldsymbol{\theta}} \frac{\delta \widehat{L}(\tau, \nu)}{\delta \nu}(\boldsymbol{\theta}, s, t) \right), \quad t \geq 0, \tag{3}$$

- The evolution of the final layer distribution $\tau(\boldsymbol{\omega})$ can be characterized as

$$\frac{\partial \tau}{\partial t}(\boldsymbol{\omega}, t) = \nabla_{\boldsymbol{\omega}} \cdot \left(\tau(\boldsymbol{\omega}, t) \nabla_{\boldsymbol{\omega}} \frac{\delta \widehat{L}(\tau, \nu)}{\delta \tau}(\boldsymbol{\omega}, t) \right), \quad t \geq 0\,, \tag{4}$$

where the functional derivative

$$\frac{\delta \widehat{L}(\tau, \nu)}{\delta \tau}(\boldsymbol{\omega}) = \mathbb{E}_{\boldsymbol{x} \sim \mathcal{D}_n} [\beta \cdot (f_{\tau,\nu}(\boldsymbol{x}) - y(\boldsymbol{x})) \cdot h(\boldsymbol{Z}_\nu(\boldsymbol{x}, 1), \boldsymbol{\omega})]\,.$$

Gram Matrix

- We define one Gram matrix for the ResNet layers, $\boldsymbol{G}_1(\tau,\nu)$ by

$$\boldsymbol{G}_1(\tau,\nu) = \int_0^1 \boldsymbol{G}_1(\tau,\nu,s)\mathrm{d}s$$
$$\boldsymbol{G}_1(\tau,\nu,s) = \mathbb{E}_{\boldsymbol{\theta}\sim\nu(\cdot,s)} \boldsymbol{J}_1(\tau,\nu,\boldsymbol{\theta},s)\boldsymbol{J}_1(\tau,\nu,\boldsymbol{\theta},s)^\top .$$

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- We define the Gram matrix for the MLP parameter distribution τ, $\boldsymbol{G}_2(\tau,\nu)$ by $\boldsymbol{G}_2(\tau,\nu) = \mathbb{E}_{\boldsymbol{\omega}\sim\tau(\cdot)} \boldsymbol{J}_2(\nu,\boldsymbol{\omega})\boldsymbol{J}_2(\nu,\boldsymbol{\omega})^\top$, where the row vector of $\boldsymbol{J}_2$ is defined as

$$(\boldsymbol{J}_2(\nu,\boldsymbol{\omega}))_{i,\cdot} = \nabla_{\boldsymbol{\omega}} h(\boldsymbol{Z}_\nu(\boldsymbol{x}_i,1),\boldsymbol{\omega}), \quad 1 \le i \le n .$$

- The Gram matrix for the whole network is $\boldsymbol{G} = \alpha^2 \boldsymbol{G}_1 + \boldsymbol{G}_2$.

Minimum Eigenvalue

Lemma

There exist a constant $\Lambda := \Lambda(d)$*, only depending on the dimension* d*, such that* $\lambda_{\min}[\boldsymbol{G}(\tau_0, \nu_0)]$ *is lower bounded by*

$$\lambda_0 := \lambda_{\min}(\boldsymbol{G}(\tau_0, \nu_0)) \geq \lambda_{\min}(\boldsymbol{G}_2(\tau_0, \nu_0)) \geq \Lambda(d)\,.$$

Theorem

Assume the PDE Eqn. 4 has solution $\tau_t \in \mathcal{P}^2$*, and the PDE Eqn. 3 has solution* $\nu_t \in \mathcal{C}(\mathcal{P}^2; [0,1])$*. Under Assumption 1, 2, 3, for some constant* C_{KL} *dependent on* d, α*, taking* $\bar{\beta} := \frac{\beta}{n} > \frac{4\sqrt{C_{\mathrm{KL}}(d,\alpha)}}{\Lambda r_{\max}}$*, the following results hold for all* $t \in [0, \infty)$*:*

$$\widehat{L}(\tau_t, \nu_t) \leq e^{-\frac{\beta^2 \Lambda}{2n} t} \widehat{L}(\tau_0, \nu_0), \quad \mathrm{KL}(\tau_t \| \tau_0) \leq \frac{C_{\mathrm{KL}}(d,\alpha)}{\Lambda^2 \bar{\beta}^2}, \quad \mathrm{KL}(\nu_t \| \nu_0) \leq \frac{C_{\mathrm{KL}}(d,\alpha)}{\Lambda^2 \bar{\beta}^2}\,.$$

where the radius $r_{\max}$ *is defined such that if* $\nu \in \mathcal{C}(\mathcal{P}^2; [0,1]), \tau \in \mathcal{P}^2$, $\max\{\mathcal{W}_2(\nu, \nu_0), \mathcal{W}_2(\tau, \tau_0)\} \leq r_{\max}$*, we have* $\lambda_{\min}(\boldsymbol{G}_2(\tau, \nu)) \geq \frac{\lambda_0}{2}$.

Generalization

Theorem (Generalization)

Assume $\tau_y \in \mathcal{C}(\mathcal{P}^2; [0,1])$ *and* $\nu_y \in \mathcal{P}^2$ *be the ground truth distributions, such that,* $y(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{\omega}\sim\tau_y} h(\boldsymbol{Z}_{\nu_y}(\boldsymbol{x}, 1), \boldsymbol{\omega})$. *Under the Assumption 1, 2 and 3, we set* $\beta > \Omega(\sqrt{n})$. *For any* $\delta > 0$, *with probability at least* $1-\delta$, *the following bound holds:*

$$\mathbb{E}_{\boldsymbol{x}\sim\mu_X} \ell_{0-1}(f_{\tau_\star,\nu_\star}(\boldsymbol{x}), y(\boldsymbol{x})) \lesssim 1/\sqrt{n} + 6\sqrt{\log(2/\delta)/2n},$$

where $\lesssim$ *hides the constant dependence on* d, α.