Kernel-Based Smoothness Analysis of Residual Networks

Tom Tirer, Joan Bruna, Raja Giryes,

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- ResNets are **superior** to MLPs in most tasks. Structural difference visible in the two NTKs?
- Provides **smoother** interpolations

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- Only very **heuristic** understanding (gradient highway) in optimization, basically **no work** on generalization

$$\underline{x}^{(l)} \longrightarrow W^{(l)}\underline{x}^{(l)} \longrightarrow V^{(l)}\phi\left(W^{(l)}\underline{x}^{(l)}\right) \longrightarrow \underline{x}^{(l)} + V^{(l)}\phi\left(W^{(l)}\underline{x}^{(l)}\right)$$

Skip connection

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where $\boldsymbol{U} \in \mathbb{R}^{d\times n}$, $\boldsymbol{W}^{(l)} \in \mathbb{R}^{n\times n}$, $\boldsymbol{V}^{(l)} \in \mathbb{R}^{n\times n}$ and $\boldsymbol{w}^{(L+1)} \in \mathbb{R}^n$

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- This function has **closed form** for *ReLU* and *erf* activation

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- $f(\cdot) \xrightarrow{(d)} \mathcal{GP}(0, \Sigma^{(L+1)})$ and kernel regression with $\Sigma^{(L+1)}$ corresponds to **Bayesian inference** with $\mathcal{GP}(0, \Sigma^{(L+1)})$ as a prior
- $\Sigma^{(L+1)}$ also arises as the **NTK** of $f(\cdot)$ if only the top layer of f is trained

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Denote by f again the output of above residual network. For width $n \to \infty$ we have:

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- Proof hence via **induction**

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- We will look at a **sequential limit** proof for presentation purposes (but bit confusing because all widths are n...)
- Proof hence via **induction**
- There are proofs **independent** of the order of limits

Proof for NNGP: Base Case

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- $L = 1$:

$$f(\boldsymbol{x}) = x_i^{(0)} = \frac{\sigma_w}{\sqrt{d}}(\boldsymbol{U}\boldsymbol{x})_i = \frac{\sigma_w}{\sqrt{d}}\sum_{k=1}^{d} U_{ik}x_k \sim \mathcal{N}(0, \sigma_w||\boldsymbol{x}||_2^2)$$

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- For the covariance we have that

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- One can easily check that Gaussianity also holds for the vector

$$(f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_m)) \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Sigma}^{(1)})$$

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Actually needs more work: $X_n \xrightarrow{(d)} X$ and $Y_n \xrightarrow{(d)} Y$ does not imply that

$X_n + Y_n \xrightarrow{(d)} X_n + Y_n$

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Seems like we need 1-homogeneous activations?

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- **Off-diagonal** terms again follow from multidimensional CLT

NTK for MLPs

Recall: For $f(\cdot)$ an MLP, we have that

$$\hat{\Theta}_{\mathrm{MLP}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = \left\langle \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{\theta}}, \frac{\partial f(\tilde{\boldsymbol{x}})}{\partial \boldsymbol{\theta}} \right\rangle \xrightarrow{(d)} \Theta_{\mathrm{MLP}}^{(L+1)}(\boldsymbol{x}, \tilde{\boldsymbol{x}})$$

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- $\Theta^{(1)}_{\text{MLP}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = \frac{\sigma_w^2}{d} \boldsymbol{x}^T \tilde{\boldsymbol{x}}$
- $\Theta^{(l+1)}_{\text{MLP}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = \Theta^{(l)}_{\text{MLP}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) \dot{\mathcal{T}}(\Sigma^{(l+1)}|_{\boldsymbol{x}, \tilde{\boldsymbol{x}}}) + \mathcal{T}(\Sigma^{(l+1)}|_{\boldsymbol{x}, \tilde{\boldsymbol{x}}})$

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For width $n \to \infty$ we have:

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  $+ \alpha^2 \sum_{m=1}^{l} \Pi^{(m)}(\boldsymbol{x}, \tilde{\boldsymbol{x}})\sigma_v^2\sigma_w^2 \mathcal{T}(\Sigma^{(m)}|_{\boldsymbol{x},\tilde{\boldsymbol{x}}})$
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where

$$\Pi^{(l)}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = \Pi^{(l+1)}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) \left(1 + \alpha^2 \sigma_v^2 \sigma_w^2 \dot{\mathcal{T}}(\Sigma^{(l+1)}(\boldsymbol{x}, \tilde{\boldsymbol{x}}))\right)$$

$$\Pi^{(L)}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = 1$$

Proof Sketch (1)

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$$\left\langle \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{\theta}}, \frac{\partial f(\tilde{\boldsymbol{x}})}{\partial \boldsymbol{\theta}} \right\rangle = \sum_{l=1}^{L} \left(\left\langle \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{W}^{(l)}}, \frac{\partial f(\tilde{\boldsymbol{x}})}{\partial \boldsymbol{W}^{(l)}} \right\rangle + \left\langle \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{V}^{(l)}}, \frac{\partial f(\tilde{\boldsymbol{x}})}{\partial \boldsymbol{V}^{(l)}} \right\rangle \right)$$
$$+ \left\langle \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{U}}, \frac{\partial f(\tilde{\boldsymbol{x}})}{\partial \boldsymbol{U}} \right\rangle + \left\langle \frac{\partial f(\underline{x})}{\partial \underline{W}^{(L+1)}}, \frac{\partial f(\tilde{\underline{x}})}{\partial \underline{W}^{(L+1)}} \right\rangle$$

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- **Recall:** $f(\boldsymbol{x}) = \frac{\sigma_w}{\sqrt{n}} \left(\boldsymbol{w}^{(L+1)} \right)^T \boldsymbol{x}^{(L)}$ and $\boldsymbol{x}^{(0)} = \frac{1}{\sqrt{d}} \boldsymbol{U}\boldsymbol{x}$

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Proof Sketch (2)

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- **Recall** the form of the residual network

$$\boldsymbol{x}^{(l+1)}(\boldsymbol{x}) = \boldsymbol{x}^{(l)}(\boldsymbol{x}) + \alpha \frac{\sigma_v}{\sqrt{n}} \boldsymbol{V}^{(l+1)} \phi\left(\frac{\sigma_w}{\sqrt{n}} \boldsymbol{W}^{(l+1)} \boldsymbol{x}^{(l)}(\boldsymbol{x})\right) \in \mathbb{R}^n$$

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- $\frac{\partial x_k^{(l)}}{\partial W_{ij}^{(l)}} = \alpha \frac{\sigma_v \sigma_w}{n} V_{ki}^{(l)} \phi'\left(g_i^{(l)}\right) x_j^{(l-1)}$

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Proof Sketch (3)

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- $\sum_{i,j=1}^{d,n} \mathbb{E}\left[\frac{\partial f(\boldsymbol{x})}{\partial U_{ij}^{(l)}} \frac{\partial f(\tilde{\boldsymbol{x}})}{\partial U_{ij}^{(l)}}\right] = \frac{1}{d} \sum_{i,j=1}^{d,n} \mathbb{E}\left[\frac{\partial f}{\partial x_i^{(0)}} x_j \frac{\partial \tilde{f}}{\partial x_i^{(0)}} \tilde{x}_j\right]$

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- $$\begin{aligned}\sum_{i,j=1}^{d,n} \mathbb{E}\left[\frac{\partial f(\boldsymbol{x})}{\partial U_{ij}^{(l)}} \frac{\partial f(\tilde{\boldsymbol{x}})}{\partial U_{ij}^{(l)}}\right] &= \frac{1}{d} \sum_{i,j=1}^{d,n} \mathbb{E}\left[\frac{\partial f}{\partial x_i^{(0)}} x_j \frac{\partial \tilde{f}}{\partial x_i^{(0)}} \tilde{x}_j\right] \\ &= \frac{1}{d} \boldsymbol{x}^T \tilde{\boldsymbol{x}} \mathbb{E}\left[\frac{\partial f}{\partial x_i^{(0)}} \frac{\partial \tilde{f}}{\partial x_i^{(0)}}\right] \\ &= \frac{K^{(1)}(\boldsymbol{x},\tilde{\boldsymbol{x}})}{\sigma_w^2} \mathbb{E}\left[\left(\boldsymbol{\delta}^{(0)}(\boldsymbol{x})\right)^T \boldsymbol{\delta}^{(0)}(\tilde{\boldsymbol{x}})\right]\end{aligned}$$

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$$= \frac{\alpha^2 \sigma_v^2}{n} \mathbb{E}\left[\delta_i^{(l)} \tilde{\delta}_i^{(l)} \mathbb{E}\left[\phi\left(g_j^{(l)}\right) \phi\left(\tilde{g}_j^{(l)}\right) \middle| \delta_i^{(l)}\right]\right]$$

Tower property: $\mathbb{E}[X] = \mathbb{E}[\mathbb{E}[X|Y]]$

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- $\sum_{i,j=1}^{d,n} \mathbb{E}\left[\frac{\partial f(\boldsymbol{x})}{\partial U_{ij}^{(l)}} \frac{\partial f(\tilde{\boldsymbol{x}})}{\partial U_{ij}^{(l)}}\right] = \frac{1}{d} \sum_{i,j=1}^{d,n} \mathbb{E}\left[\frac{\partial f}{\partial x_i^{(0)}} x_j \frac{\partial \tilde{f}}{\partial x_i^{(0)}} \tilde{x}_j\right]$
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$g_j^{(l)} \sim \mathcal{GP}(0, \Sigma^{(l)})$

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$$= \frac{\alpha^2 \sigma_v^2}{n} \underbrace{\mathcal{T}(\boldsymbol{\Sigma}^{(l)}|_{\boldsymbol{x},\tilde{\boldsymbol{x}}})}_{\text{deterministic}} \mathbb{E}\left[\delta_i^{(l)} \tilde{\delta}_i^{(l)}\right]$$

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$$= \frac{\alpha^2 \sigma_v^2}{n} \mathbb{E}\left[\delta_i^{(l)} \tilde{\delta}_i^{(l)} \mathcal{T}(\boldsymbol{\Sigma}^{(l)}|_{\boldsymbol{x}, \tilde{\boldsymbol{x}}})\right]$$

$$= \frac{\alpha^2 \sigma_v^2}{n} \mathcal{T}(\boldsymbol{\Sigma}^{(l)}|_{\boldsymbol{x}, \tilde{\boldsymbol{x}}}) \mathbb{E}\left[\delta_i^{(l)} \tilde{\delta}_i^{(l)}\right]$$

- **So:** $\left\langle \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{V}^{(l)}}, \frac{\partial f(\tilde{\boldsymbol{x}})}{\partial \boldsymbol{V}^{(l)}} \right\rangle = \frac{\alpha^2 \sigma_v^2}{n} \mathcal{T}(\boldsymbol{\Sigma}^{(l)}|_{\boldsymbol{x}, \tilde{\boldsymbol{x}}}) \mathbb{E}\left[\left(\boldsymbol{\delta}^{(l)}\right)^T \tilde{\boldsymbol{\delta}}^{(l)}\right]$

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- A similar sequence of steps leads to

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- This is given exactly by $\Pi(\boldsymbol{x}, \tilde{\boldsymbol{x}})$ in the theorem

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The paper that Seyed presented

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Time-invariance of Θ_{res}

- One can now prove that the NTK remains **constant** through training with GD
- Proof very similar to ”*Wide neural networks of any depth evolve as linear models*”
- Interesting decomposition of proof into two steps, one **dependent** on the architecture and the other **independent** of particular architecture

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- In essence, one needs to control the norm of the Jacobian and show the Lipschitzness

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Denote the training loss by $L(\boldsymbol{\theta}_t) = ||\boldsymbol{f}(\boldsymbol{\theta}_t) - \boldsymbol{y}||_2^2$ and by $\boldsymbol{\Theta} = \boldsymbol{\Theta}_{\text{res}}(\boldsymbol{X}, \boldsymbol{X})$ the kernel evaluated on the training set. Fix a learning rate $\eta_0 \leq 2(\lambda_{\min}(\boldsymbol{\Theta}) + \lambda_{\max}(\boldsymbol{\Theta}))^{-1}$. Let $n > C^2$. Then with high probability there exists $R_0, K > 0$ such that:

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Follows from Lemma **without** any architecture specific arguments!

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Reflects smoothness of f_{res} to some degree

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$$\propto \left(\boldsymbol{w}^{(L+1)} \right)^T \left(\prod_{l=1}^{L} \left(\mathbb{1} + \frac{\alpha \sigma_v}{n} \boldsymbol{V}^{(l)} diag \left(\phi' \left(\boldsymbol{g}^{(l)} \right) \right) \boldsymbol{W}^{(l)} \right) \right) \frac{\boldsymbol{U}}{\sqrt{nd}}$$

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- Bounding the norm of the derivative leads to

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Singular Values of Gaussian Random Matrices

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Lemma: *Take $\boldsymbol{W} \in \mathbb{R}^{m \times n}$ with $W_{ij} \sim \mathcal{N}(0,1)$. Then with probability $\geq 1 - 2\exp(-\frac{t^2}{2})$ it holds:*

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- Let $C = \frac{3KR_0}{\lambda_{\min}(\boldsymbol{\Theta})}$. It holds (in NTK regime) that $\boldsymbol{\theta}_t \in B(\boldsymbol{\theta}_0, C)$. We can hence arrive at

$$\begin{aligned} ||\boldsymbol{W}_t^{(l)}||_2 &\leq ||\boldsymbol{W}_0^{(l)}||_2 + ||\boldsymbol{W}_t^{(l)} - \boldsymbol{W}_0^{(l)}||_2 \\ &\leq 2\sqrt{n} + t + C \leq 3\sqrt{n} \end{aligned}$$

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- Similary we find $||\boldsymbol{U}||_2 \leq \sqrt{d} + 2\sqrt{n}$ and $||\boldsymbol{V}^{(l)}||_2 \leq 3\sqrt{n}$

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- **Observe:** Bound decreases with α. Better empirical performance has been observed for smaller α!

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- We can make a similar derivation for the MLP:

$$\left\| \frac{\partial f_{\mathsf{MLP}}(\boldsymbol{x})}{\partial \boldsymbol{x}} \right\|_2 \leq 2C_\phi \left(1 + 2\sqrt{\frac{n}{d}}\right) (3C_\phi)^{L-1} = B_{\mathsf{MLP}}$$

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- Comparing the two bounds shows:

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- We can hence obtain **smoother** interpolations by using $\alpha = 0.1$ for any depth. Apparently values on this order also work best **in practice**!

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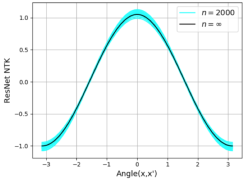
- Calculate norm as

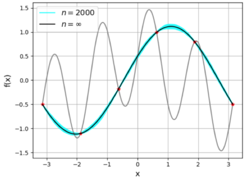
Fourier transform

$$||f||_{\text{Gauss}} = \frac{1}{(2\phi)^{\frac{1}{d}}} \int \frac{|\mathcal{F}[f](\omega)|^2}{\mathcal{F}[K_{\text{Gauss}}](\omega)} d\omega$$

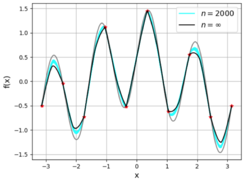
Experiments (I)



(a) Empirical and asymptotic NTK



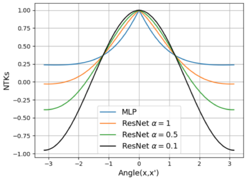
(b) Interpolation with 6 samples



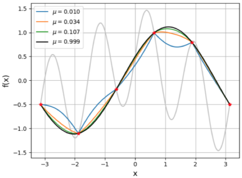
(c) Interpolation with 10 samples

Finite (black) versus infinite width ResNet (blue). In a) the two kernels are compared, in b) and c) the predictive functions with different learning rates. Empirical results perfectly **agree** with the predictions of theory.

Experiments (II)



(a) NTKs (normalized to unit peak)
$L = 5$



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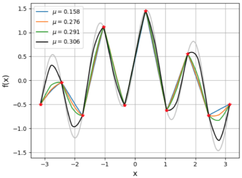

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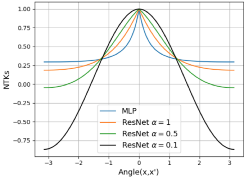
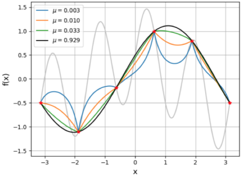
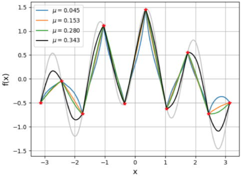


(d) NTKs (normalized to unit peak)
$L = 15$



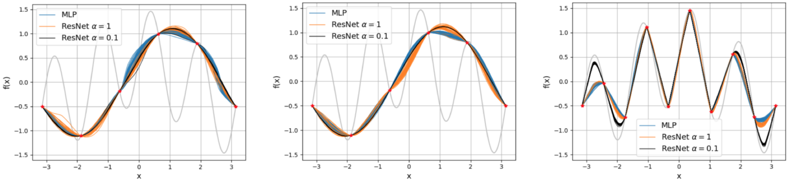
(e) Interpolation with 6 samples
$L = 15$



(f) Interpolation with 10 samples
$L = 15$

MLP (black) and Resnets for different α's and different number of layers. Visually, fits become smoother with **smaller** α. μ-measure agrees with that observation.

Experiments (III)



Same visualizations **out of** the NTK regime (lazy regime), meaning **smaller** width $n = 500$, **Xavier** initialization (no $\frac{1}{\sqrt{n}}$) and different (**adaptive**) optimizers. Same observations roughly hold in this regime, ResNet is smoother than MLP and decreasing α promotes smoothness.

Discussion

- Notions of smoothness seem interesting and the bounds are rather easy. Maybe one can do something in the spirit of **norm-based generalization bounds** but for trained networks instead of all networks (avoiding the union bound because we have roughly a bound on Lipschitz constant of trained network)
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