On the linearity of large non-linear models: when and why the tangent kernel is constant

Chaoyue Liu, Libin Zhu, Mikhail Belkin,

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- Revisiting of the proof that neural tangent kernel remains **constant** during training
- Conceptually **easier** reasoning when and why NTK is constant
- **Lazy training** is not the origin of constancy, it’s a consequence of the architecture!

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  where $\boldsymbol{W}^{(l)} \in \mathbb{R}^{m_{l-1}\times m_l}$ and $\sigma : \mathbb{R} \to \mathbb{R}$ some **non-linearity**
- The final output is given by

$$f(\boldsymbol{x}) = \frac{1}{\sqrt{m}}\boldsymbol{v}^T\boldsymbol{\alpha}^{(L)}(\boldsymbol{x})$$

  where $\boldsymbol{v} \in \mathbb{R}^m$ is **not** trainaible

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- β-smooth: $||\sigma(\boldsymbol{w}) - \sigma(\boldsymbol{v}) - \nabla\sigma(\boldsymbol{v})(\boldsymbol{w} - \boldsymbol{v})||_2 \leq \frac{\beta}{2}||\boldsymbol{w} - \boldsymbol{v}||_2^2$

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- Lipschitz: $||\sigma(\boldsymbol{w}) - \sigma(\boldsymbol{v})||_2 \leq \gamma||\boldsymbol{v} - \boldsymbol{w}||_2$

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$$K_{\boldsymbol{w}}(\boldsymbol{x}, \boldsymbol{x}') = \left(\nabla_{\boldsymbol{w}} f(\boldsymbol{w}; \boldsymbol{x})\right)^T \nabla_{\boldsymbol{w}} f(\boldsymbol{w}; \boldsymbol{x}')$$

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- Of particular interest are diagonal entries:

$$K_{\boldsymbol{w}}(\boldsymbol{x}, \boldsymbol{x}) = ||\nabla_{\boldsymbol{w}} f(\boldsymbol{w}; \boldsymbol{x})||_2^2$$

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Constancy $\iff$ Linear

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Proof is surprisingly long but uses very elementary tools from calculus.

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- **Now:** $\Longrightarrow$ $f(\boldsymbol{w}, \boldsymbol{x})$ linear $\Longrightarrow$ $K_{\boldsymbol{w}}$ constant

Let us hence first show that $f(\boldsymbol{w}; \boldsymbol{x})$ becomes linear.

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Linearity vs Hessian

A differentiable function $f : \mathbb{R}^d \to \mathbb{R}$,$\boldsymbol{w} \mapsto f(\boldsymbol{w})$ is linear if and only if the Hessian $\boldsymbol{H}_f = \frac{\partial f}{\partial \boldsymbol{w}^2}$ vanishes $\forall \boldsymbol{w} \in \mathbb{R}^d$.

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It hence suffices to show that $\boldsymbol{H}_f = 0$ for $m \to \infty$ or equivalently $||\boldsymbol{H}_f||_2 = 0$

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$$\left| K_{\boldsymbol{w}}(\boldsymbol{x}, \boldsymbol{x}') - K_{\boldsymbol{w}_0}(\boldsymbol{x}, \boldsymbol{x}') \right| = \mathcal{O}(R\epsilon)$$

$\forall \boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^{m_0}$ and $\forall \boldsymbol{w} \in \mathcal{B}(\boldsymbol{w}_0, R)$

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Hence if $\epsilon = \epsilon(m) \xrightarrow{m \to \infty} 0$ then also

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Take NN $f(\boldsymbol{w}; \boldsymbol{x})$ and consider β-smooth and $\mu - PL^*$ loss $L(\boldsymbol{w})$. Fix $R = \frac{2\sqrt{2\beta L(\boldsymbol{w}_0)}}{\mu}$. Then it holds that:

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Thus: Fixing $R = \frac{2\sqrt{2\beta L(\boldsymbol{w}_0)}}{\mu}$ above (independent of m) **suffices**!

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Thus: $||\boldsymbol{H}||_2 \xrightarrow{m \to \infty} 0$

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Moreover:

$$K_{\boldsymbol{w}}(\boldsymbol{x}, \boldsymbol{x}) = x^2\frac{1}{m}\sum_{i=1}^{m}\sigma'(w_i x)$$

Diagonal Kernel Entry $K_{\boldsymbol{w}}(x, x)$

On the other hand we have that:

$$\frac{\partial f}{\partial w_i} = \frac{\partial}{\partial w_i} \frac{1}{\sqrt{m}} \sum_{k=1}^{m} v_k \sigma(w_k x) = \frac{1}{\sqrt{m}} v_i \sigma'(w_i x) x$$

Thus:

$$||\nabla f(\boldsymbol{w}, x)||_2^2 = \frac{x^2}{m} \sum_{i=1}^{m} v_i^2 \sigma'(w_i x) = \frac{x^2}{m} \sum_{i=1}^{m} \sigma'(w_i x) = \Theta(1)$$

Moreover:

$$K_{\boldsymbol{w}}(\boldsymbol{x}, \boldsymbol{x}) = x^2 \frac{1}{m} \sum_{i=1}^{m} \sigma'(w_i x) \xrightarrow{m \to \infty} x^2 \mathbb{E}_{w \sim \mathcal{N}(0,1)}[\sigma'(w_i x)]$$

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- We have the following easy consequence of Hölder inequality:

Given $\boldsymbol{T} \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ and $\boldsymbol{v} \in \mathbb{R}^{d_3}$, consider $A_{ij} = \sum_k T_{ijk} v_k$.
It holds that

$$||\boldsymbol{A}||_2 \leq ||\boldsymbol{T}||_{2,2,1} ||\boldsymbol{v}||_\infty$$

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$$f(\boldsymbol{x}) = \frac{1}{\sqrt{m}} \boldsymbol{v}^T \boldsymbol{\alpha}^{(L)}(\boldsymbol{x})$$

  where $\boldsymbol{v} \in \mathbb{R}^m$ is **not** trainable

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Bound on Hessian

We have the following bound on the norm of the Hessian:

$$||\boldsymbol{H}||_2 \le C_1 \mathcal{Q}_{2,2,1} \mathcal{Q}_\infty + \frac{1}{\sqrt{m}} C_2 \mathcal{Q}_2$$

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- Namely, using the 1-dim 1-hidden layer network $f(\boldsymbol{w}; x)$ as

$$\tilde{f}(\boldsymbol{w}, x) = \phi(f(\boldsymbol{w}; x))$$

where $\phi : \mathbb{R} \to \mathbb{R}$ is some twice-differentiable non-linearity

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- Let's look at the Hessian:

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$$= \phi''(f)\frac{\partial f}{\partial w_i}\frac{\partial f}{\partial w_j} + \phi'(f)\frac{\partial^2 f}{\partial w_j \partial w_i}$$

- **Thus:** $\tilde{\boldsymbol{H}} = \phi''(f)\left(\nabla_{\boldsymbol{w}} f\right)\left(\nabla_{\boldsymbol{w}} f\right)^T + \phi'(f)\boldsymbol{H}$

- From **Weyl's**-inequality we have that for all symmetric matrices $\boldsymbol{A} = \boldsymbol{B} + \boldsymbol{C}$:

$$\lambda_1(\boldsymbol{A}) \geq \lambda_1(\boldsymbol{B}) + \lambda_n(\boldsymbol{C}) \iff ||\boldsymbol{A}||_2 \geq ||\boldsymbol{B}||_2 - ||\boldsymbol{C}||_2$$

- Applying this to $\tilde{\boldsymbol{H}}$ leads to

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- **Thus**, as long as ϕ'' doesn't vanish (so if not linear) we have

$$||\tilde{\boldsymbol{H}}||_2 = \Omega(1)$$

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- This "kills" the $\frac{1}{\sqrt{m}}$ from before!

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- Well-conditionedness is somewhat **"passed"** on to the non-linear output model from the linear output model. That's why these models also converge fast in practice.

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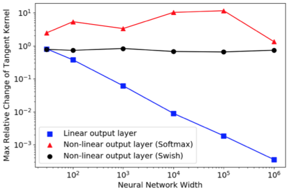

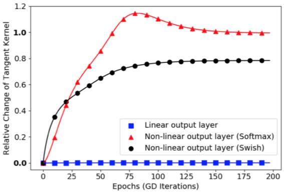

Change in NTK for **linear** versus **non-Linear** output activation. 1 hidden layer network with either linear, softmax or swish activation at output.

Experiments (II)

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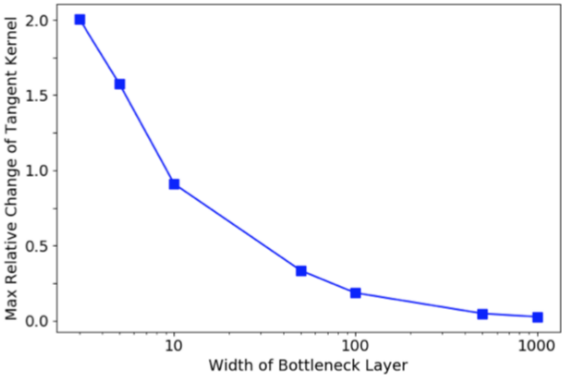

Width of the bottleneck layer and corresponding change in NTK.
3 hidden layer network of widths $m = 10^4$

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- Are similar results known for SGD, ADAM, second order methods? What does it take to fall out of this ball (except for big learning rates)?