Infinitely Wide Nets

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Introduction

(Real) neural nets are hard to study theoretically:

1. Non-convex optimization landscape;
2. Non-deterministic training procedure;
3. Existence of poorly-generalizing minima [Zhang et al., 2016].

What can we do:

1. Come up with a theoretically-tractable proxy-model;
2. Relate a real net to this proxy.

Consider a neural net training process; **hyperparameters are:**

1. Learning rate;
2. Batch size;
3. Depth ($\propto$ number of dense/conv layers);
4. Width ($\propto$ number of hidden neurons);
5. ...

Taking a limit wrt to each of these hyperparameters may simplify the model:

1. Learning rate $\to 0 \Rightarrow$ continuous-time GD;
2. Batch size $\to \infty \Rightarrow$ deterministic GD;
3. Depth $\to \infty \Rightarrow$ ODENet (?) [Chen et al., 2018];
4. Width $\to \infty \Rightarrow$ **our topic today.**

There are **multiple infinite-width limits:**

1. A (constant) NTK limit: [Jacot et al., 2018];
2. A mean-field limit: multiple works.[1]

The cause of difference is **a hyperparameter scaling.**

Questions:

1. What are the properties of these limits (convergence/generalization)?
2. Other infinite-width limits?
3. Which of the limits is the best proxy-model for a finite-width net?

[1] [Mei et al., 2018, Mei et al., 2019, Rotskoff and Vanden-Eijnden, 2019, Chizat and Bach, 2018, Sirignano and Spiliopoulos, 2020, Yarotsky, 2018]

NTK limit

Consider a model $f(\mathbf{x}; \theta)$;
we minimize a loss $\mathcal{L}(\theta) = \mathbb{E}_{\mathbf{x},y} \ell(y, f(\mathbf{x}; \theta))$ with GD:

$$\dot{\theta}_t = -\eta \mathbb{E}_{\mathbf{x},y} \left. \frac{\partial \ell(y, z)}{\partial z} \right|_{z = f(\mathbf{x}; \theta_t)} \nabla_\theta f(\mathbf{x}; \theta_t); \qquad \theta_0 \sim \mathcal{P}_{init}.$$

This implies **a kernel gradient descent:**

$$\dot{f}_t(\mathbf{x}') = \nabla_\theta^T f(\mathbf{x}'; \theta_t) \dot{\theta}_t = -\eta \mathbb{E}_{\mathbf{x},y} \left. \frac{\partial \ell(y, z)}{\partial z} \right|_{z = f(\mathbf{x}; \theta_t)} K_t(\mathbf{x}', \mathbf{x}); \quad f_0 \sim \mathcal{F}_{init}.$$

Here we have introduced **a neural tangent kernel (NTK):**

$$K_t(\mathbf{x}', \mathbf{x}) = \nabla_\theta^T f(\mathbf{x}'; \theta_t) \nabla_\theta f(\mathbf{x}; \theta_t).$$

Note:

1. All info about the weights is "hidden" inside the kernel;
2. NTK is generally stochastic and evolves with time.

First consider a model with L hidden layers of width d in **default parameterization:**

$$f_{def}(\mathbf{x};\theta) = \sum_{r_L=1}^{d} \theta^L_{r_L} \phi\left(\dots \sum_{r_1=1}^{d} \theta^1_{r_2 r_1} \phi\left(\theta^{in,T}_{r_1} \mathbf{x}\right)\right).$$

The training process is:

$$\dot{\theta}_t = -\eta \mathbb{E}_{\mathbf{x},y} \left.\frac{\partial \ell(y,z)}{\partial z}\right|_{z=f_{def}(\mathbf{x};\theta_t)} \nabla_\theta f_{def}(\mathbf{x};\theta_t);$$

$$\theta^{in}_{r_1;0} \sim \mathcal{N}(0, I), \quad \theta^l_{r_{l+1},r_l;0} \sim \mathcal{N}(0, d^{-1}) \quad \forall l \in [L].$$

Up to a constant factor, the network is initialized with **He initialization scheme.**[2]

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[2][He et al., 2015]

Consider then the same model in **NTK parameterization:**

$$f_{ntk}(\mathbf{x};\theta) = d^{-1/2}\sum_{r_L=1}^{d}\theta^{L}_{r_L}\phi\left(\dots d^{-1/2}\sum_{r_1=1}^{d}\theta^{1}_{r_2 r_1}\phi\left(\theta^{in,T}_{r_1}\mathbf{x}\right)\right).$$

The training process is:

$$\dot{\theta}_t = -\eta\mathbb{E}_{\mathbf{x},y}\left.\frac{\partial\ell(y,z)}{\partial z}\right|_{z=f_{ntk}(\mathbf{x};\theta_t)}\nabla_\theta f_{ntk}(\mathbf{x};\theta_t);$$

$$\theta^{in}_{r_1;0}\sim\mathcal{N}(0,I),\quad \theta^{l}_{r_{l+1},r_l;0}\sim\mathcal{N}(0,1)\quad \forall l\in[L].$$

Important:

1. The initialization does not depend on d now;
2. The initial model didn't change but the training process did: $f_{ntk;0} = f_{def;0}$ **but** $f_{ntk;t} \neq f_{def;t}\ \forall t > 0$;
3. **The NTK converges to a constant deterministic kernel:** $\lim_{d\to\infty} K_t(\mathbf{x}',\mathbf{x}) = \mathbb{E}\, K_0(\mathbf{x}',\mathbf{x})$.

For the sake of illustration, consider $L = 1$ with NTK parameterization:

$$f_{ntk}(\mathbf{x}; \mathbf{a}, W) = d^{-1/2} \sum_{r=1}^{d} a_r \phi(\mathbf{w}_r^T \mathbf{x}).$$

$$\dot{a}_{r;t} = -\eta \mathbb{E} \left. \frac{\partial \ell(y, z)}{\partial z} \right|_{z = f_{ntk}(\mathbf{x}; \mathbf{a}_t, W_t)} d^{-1/2} \phi(\mathbf{w}_{r;t}^T \mathbf{x}), \quad a_{r;0} \sim \mathcal{N}(0, 1);$$

$$\dot{\mathbf{w}}_{r;t} = -\eta \mathbb{E} \left. \frac{\partial \ell(y, z)}{\partial z} \right|_{z = f_{ntk}(\mathbf{x}; \mathbf{a}_t, W_t)} d^{-1/2} a_{r;t} \phi'(\mathbf{w}_{r;t}^T \mathbf{x}) \mathbf{x}, \quad \mathbf{w}_{r;0} \sim \mathcal{N}(0, I).$$

Note: $\dot{a}_{r;t}$ and $\dot{\mathbf{w}}_{r;t}$ go to zero as $d \to \infty$.

Hence **the weights do not evolve in the limit.**

$$
\begin{aligned}
K_t(\mathbf{x}', \mathbf{x}) = \nabla_{\mathbf{a}}^T f(\mathbf{x}'; \mathbf{a}_t, W_t) \nabla_{\mathbf{a}} f(\mathbf{x}; \mathbf{a}_t, W_t) + \\
+ \operatorname{tr}(\nabla_W^T f(\mathbf{x}'; \mathbf{a}_t, W_t) \nabla_W f(\mathbf{x}; \mathbf{a}_t, W_t)) = \\
= d^{-1} \sum_{r=1}^{d} \left(\phi(\mathbf{w}_{r;t}^T \mathbf{x}') \phi(\mathbf{w}_{r;t}^T \mathbf{x}) + |a_{r;t}|^2 \phi'(\mathbf{w}_{r;t}^T \mathbf{x}') \phi'(\mathbf{w}_{r;t}^T \mathbf{x}) \mathbf{x}'^{,T} \mathbf{x} \right) \to \\
\to \mathbb{E}_{(a, \mathbf{w}) \sim \mathcal{N}(0, I)} \left(\phi(\mathbf{w}^T \mathbf{x}') \phi(\mathbf{w}^T \mathbf{x}) + |a|^2 \phi'(\mathbf{w}^T \mathbf{x}') \phi'(\mathbf{w}^T \mathbf{x}) \mathbf{x}'^{,T} \mathbf{x} \right) \neq 0.
\end{aligned}
$$

The NTK converges to a constant deterministic kernel due to LLN.

For comparison consider $L = 1$ with default parameterization:

$$f_{def}(\mathbf{x}; \mathbf{a}, W) = \sum_{r=1}^{d} a_r \phi(\mathbf{w}_r^T \mathbf{x}).$$

$$\dot{a}_{r;t} = -\eta \mathbb{E}\ \left.\frac{\partial \ell(y,z)}{\partial z}\right|_{z=f_{def}(\mathbf{x};\mathbf{a}_t,W_t)} \phi(\mathbf{w}_{r;t}^T \mathbf{x}), \quad a_{r;0} \sim \mathcal{N}(0, d^{-1});$$

$$\dot{\mathbf{w}}_{r;t} = -\eta \mathbb{E}\ \left.\frac{\partial \ell(y,z)}{\partial z}\right|_{z=f_{def}(\mathbf{x};\mathbf{a}_t,W_t)} a_{r;t} \phi'(\mathbf{w}_{r;t}^T \mathbf{x}) \mathbf{x}, \quad \mathbf{w}_{r;0} \sim \mathcal{N}(0, I).$$

Now $\dot{a}_{r;t}$ and $\dot{\mathbf{w}}_{r;t}$ **do not go to zero** as $d \to \infty$.

$$K_t(\mathbf{x}', \mathbf{x}) = \sum_{r=1}^{d} \left(\phi(\mathbf{w}_{r;t}^T \mathbf{x}') \phi(\mathbf{w}_{r;t}^T \mathbf{x}) + |a_{r;t}|^2 \phi'(\mathbf{w}_{r;t}^T \mathbf{x}') \phi'(\mathbf{w}_{r;t}^T \mathbf{x}) \mathbf{x}'^{,T} \mathbf{x} \right).$$

The kernel diverges at initialization: $K_0(\mathbf{x}', \mathbf{x}) \to \infty$.

Consider a model f_d of width d with **NTK parameterization.**

Theorem (convergence to a limit model; [Jacot et al., 2018])
For sufficiently regular ϕ $K_{d,t} \to K_\infty = \mathbb{E}\, K_{d,0}$ and $f_{d,t} \to f_{\infty,t}$ as $d \to \infty$, where limit dynamics is given as:

$$\dot{f}_{\infty,t}(\mathbf{x}') = -\eta \mathbb{E}_{\mathbf{x},y} \left. \frac{\partial \ell(y,z)}{\partial z} \right|_{z=f_{\infty,t}(\mathbf{x})} K_\infty(\mathbf{x}',\mathbf{x}), \quad f_{\infty,0}(\mathbf{x}) \sim \mathcal{N}(0, \sigma_0^2(\mathbf{x})).$$

Question: what is the limit model for the default parameterization?
We shall discuss it later on.[3]

[3] or, see [Golikov, 2020a].

Suppose we have a train dataset of size n: $S_n = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$. Assume:

1. l_2 loss: $\ell(y, z) = \frac{1}{2}|y - z|^2$;
2. The Gramian $G = \{K_\infty(\mathbf{x}_i, \mathbf{x}_j)\}_{i,j=1}^n$ is positive definite.

Then $f_{\infty,t}$ **converges to a global minimum on the train dataset.**

Indeed, consider l_2-regression:

$$\dot{f}_{\infty,t}(\mathbf{x}) = \eta \frac{1}{n} \sum_{j=1}^{n} (y_j - f_{\infty,t}(\mathbf{x}_j)) K_\infty(\mathbf{x}, \mathbf{x}_j).$$

Denote $\mathbf{y} = \{y_i\}_{i=1}^n$, $\hat{\mathbf{y}}_t = \{f_{\infty,t}(\mathbf{x}_i)\}_{i=1}^n$.

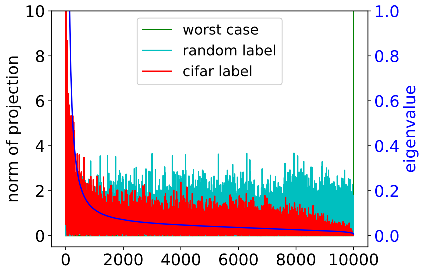
Let $\{(\lambda_i, \mathbf{v}_i)\}_{i=1}^n$ be a set of eigenvalue-eigenvector pairs for G. Then (see [Arora et al., 2019b]):

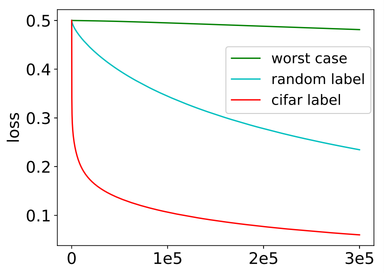
$$\|\hat{\mathbf{y}}_t - \mathbf{y}\|_2^2 = \sum_{i=1}^{n} ((\hat{\mathbf{y}}_0 - \mathbf{y})^T \mathbf{v}_i)^2 e^{-\frac{2\eta}{n} \lambda_i t}.$$

Important: assuming $\hat{\mathbf{y}}_0 = 0$, the speed of convergence is related to a **spectrum alignment** $\{(\mathbf{y}^T \mathbf{v}_i)^2\}_{i=1}^n$.

$$\|\hat{\mathbf{y}}_t - \mathbf{y}\|_2^2 = \sum_{i=1}^{n} (\mathbf{y}^T \mathbf{v}_i)^2 e^{-\frac{2\eta}{n}\lambda_i t}.$$

Norm of projection: $\mathbf{y}^T\mathbf{v}_i$; eigenvalue: λ_i.





So far, we have two results:

1. A finite-width model converges to a limit one as $d \to \infty$;
2. A limit model converges to a global minimum as $t \to \infty$ (**asymptotic convergence guarantee**).

Theorem (non-asymptotic conv. guarantee; [Du et al., 2018])
Consider a two-layered network with ReLU activations.

$\exists C$: *for* $\delta > 0$ *and* $d \geq C \frac{n^6}{\delta^3 \lambda_n^4}$ *(large but finite width)*

$$\|\hat{\mathbf{y}}_t - \mathbf{y}\|_2^2 \leq \exp\left(-\frac{2\eta}{n} \lambda_n t\right) \quad \textit{w.p.} \geq 1 - \delta.$$

[Song and Yang, 2019]: the same guarantee for $d \geq C \frac{n^4}{\lambda_n^4} \log^3\left(\frac{n}{\delta}\right)$.
[Arora et al., 2019b]: a similar guarantee for the spectrum alignment.

- Consider l_1 loss: $\ell(y, z) = |y - z|$.
- Assume $f_0 \equiv 0$.
- Suppose we have converged to a zero loss on the dataset $S_n = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ sampled from $\mathcal{D}$. Let $\hat{f}_n$ be the final network.

Theorem (non-asymptotic generalization guarantee; [Arora et al., 2019b])
Consider a two-layered network with ReLU activations.

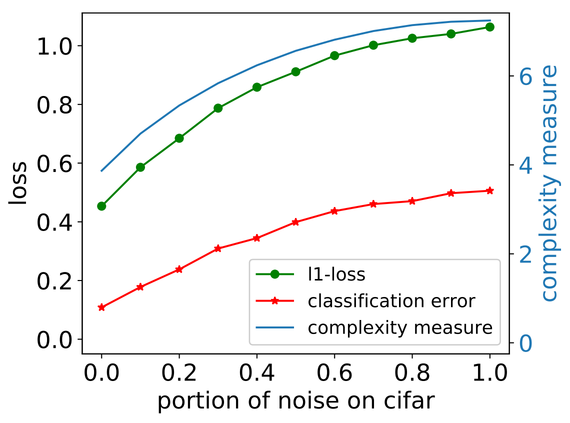
Then given $\delta \in (0, 1)$ for sufficiently large d w.p. $\geq 1 - \delta$ over S_n and initialization

$$\mathbb{E}_{\mathbf{x}, y \sim \mathcal{D}} \ell(y, \hat{f}_n(\mathbf{x})) \leq \sqrt{\frac{2\mathbf{y}^T G^{-1} \mathbf{y}}{n}} + O\left(\sqrt{\frac{\log \frac{n}{\lambda_n \delta}}{n}}\right).$$

Intuition: if we train a network on a dataset that aligns well with NTK then our network generalizes well w.h.p.

$$\mathbb{E}_{\mathcal{D}}\ell(y, \hat{f}_n(\mathbf{x})) \leq \sqrt{\frac{2\mathbf{y}^T G^{-1}\mathbf{y}}{n}} + O\left(\sqrt{\frac{\log \frac{n}{\lambda_n \delta}}{n}}\right) \text{ w.p. } \geq 1 - \delta.$$

A complexity measure: $\sqrt{2\mathbf{y}^T G^{-1}\mathbf{y}/n}$.



Recall the definition of NTK:

$$K_\infty(\mathbf{x}', \mathbf{x}) = \mathbb{E}_{\theta_0} K_0(\mathbf{x}', \mathbf{x}) = \mathbb{E}_{\theta_0} \nabla_\theta^T f(\mathbf{x}'; \theta_0) \nabla_\theta f(\mathbf{x}; \theta_0).$$

How to compute it?

1. Via Monte-Carlo [Lee et al., 2019]:
   - +: applicable to any architecture;
   - -: noisy.
2. Analytically [Arora et al., 2019a]:
   - +: exact and efficient;
   - -: available only for ReLU FC and Conv nets w/o BNs etc.

Depth	CNN	CNTK
3	63.81%	**70.47%**
4	**80.93%**	75.93%
6	**83.75%**	76.73%
11	**82.92%**	77.43%
21	**83.30%**	77.08%

Table 1: Comparing deep CNNs trained with square loss with their constant-kernel counterparts [Arora et al., 2019a]. **Dataset:** CIFAR10.

Conclusion: if we fix the kernel, performance gets worse.

Hence the kernel evolution is important.

Mean-field limit

Consider **a neural net with a single hidden layer:**

$$f_d(\mathbf{x}) = \frac{1}{d} \sum_{r=1}^{d} a_r \phi(\mathbf{w}_r^T \mathbf{x}).$$

Note the factor d^{-1} instead of $d^{-1/2}$ (NTK) or d^0 (default).

The training process is:

$$\dot{a}_{r;t} = -\eta \mathbb{E} \left. \frac{\partial \ell(y,z)}{\partial z} \right|_{z=f_{d,t}(\mathbf{x})} d^{-1} \phi(\mathbf{w}_{r;t}^T \mathbf{x}), \quad a_{r;0} \sim \mathcal{N}(0,1);$$

$$\dot{\mathbf{w}}_{r;t} = -\eta \mathbb{E} \left. \frac{\partial \ell(y,z)}{\partial z} \right|_{z=f_{d,t}(\mathbf{x})} d^{-1} a_{r;t} \phi'(\mathbf{w}_{r;t}^T \mathbf{x}) \mathbf{x}, \quad \mathbf{w}_{r;0} \sim \mathcal{N}(0,I).$$

Take $\eta = \eta^* d$. Then $\dot{a}_{r;t}$ and $\dot{\mathbf{w}}_{r;t}$ do not go to zero as $d \to \infty$.
Hence the weights evolve.

Consider **a weight-space measure:**

$$\mu_d = d^{-1} \sum_{r=1}^{d} \delta_{a_r} \otimes \delta_{\mathbf{w}_r} \in \mathcal{M}(\mathbb{R}^{1+d_{\mathbf{x}}}).$$

We can express the model in terms of this measure:

$$f_d(\mathbf{x}) = \int a\phi(\mathbf{w}^T \mathbf{x})\, \mu_d(da, d\mathbf{w}).$$

Also, express the training process [Rotskoff and Vanden-Eijnden, 2019]:

$$\dot{\mu}_{d,t} = -\eta^* \operatorname{div}(\mu_{d,t} \mathbf{v}_{d,t}), \quad \mu_{d,0} = d^{-1} \sum_{r=1}^{d} \delta_{a_{r;0}} \otimes \delta_{\mathbf{w}_{r;0}},$$

$$\mathbf{v}_{d,t}(a, \mathbf{w}) = \mathbb{E}_{\mathbf{x},y} \left.\frac{\partial \ell(y, z)}{\partial z}\right|_{z = f_{d,t}(\mathbf{x})} [\phi(\mathbf{w}^T \mathbf{x}), a\phi'(\mathbf{w}^T \mathbf{x})\mathbf{x}^T]^T.$$

Important: the weights are now "hidden" inside the measure.

The initial measure is random:

$$\mu_{d,0} = d^{-1} \sum_{r=1}^{d} \delta_{a_{r;0}} \otimes \delta_{\mathbf{w}_{r;0}}, \quad \delta_{a_{r;0}} \sim \mathcal{N}(0,1),\ \delta_{\mathbf{w}_{r;0}} \sim \mathcal{N}(0, I_{d_{\mathbf{x}}}) \quad \forall r \in [d].$$

However **it converges to a deterministic one:**

$$\lim_{d \to \infty} \mu_{d,0} = \mu_{\infty,0} = \mathcal{N}(0, I_{1+d_{\mathbf{x}}}).$$

This gives the limit dynamics:

$$\dot{\mu}_{\infty,t} = -\eta^* \operatorname{div}(\mu_{\infty,t} \mathbf{v}_{\infty,t}), \quad \mu_{\infty,0} = \mathcal{N}(0, I_{1+d_{\mathbf{x}}}),$$

$$\mathbf{v}_{\infty,t}(a, \mathbf{w}) = \mathbb{E}_{\mathbf{x},y} \left. \frac{\partial \ell(y,z)}{\partial z} \right|_{z=f_{\infty,t}(\mathbf{x})} [\phi(\mathbf{w}^T \mathbf{x}), a\phi'(\mathbf{w}^T \mathbf{x}) \mathbf{x}^T]^T,$$

$$f_{\infty,t}(\mathbf{x}) = \int a\phi(\mathbf{w}^T \mathbf{x})\, \mu_{\infty,t}(da, d\mathbf{w}).$$

This limit is referred as **the mean-field limit.**

What happens to the kernel in the mean-field limit?

$$K_t(\mathbf{x}', \mathbf{x}) = \eta \nabla_{\mathbf{a}}^T f(\mathbf{x}'; \mathbf{a}_t, W_t) \nabla_{\mathbf{a}} f(\mathbf{x}; \mathbf{a}_t, W_t) +$$

$$+ \eta \operatorname{tr}(\nabla_W^T f(\mathbf{x}'; \mathbf{a}_t, W_t) \nabla_W f(\mathbf{x}; \mathbf{a}_t, W_t)) =$$

$$= \eta^* d^{-1} \sum_{r=1}^{d} \left(\phi(\mathbf{w}_{r;t}^T \mathbf{x}') \phi(\mathbf{w}_{r;t}^T \mathbf{x}) + |a_{r;t}|^2 \phi'(\mathbf{w}_{r;t}^T \mathbf{x}') \phi'(\mathbf{w}_{r;t}^T \mathbf{x}) \mathbf{x}'^{,T} \mathbf{x} \right) \to$$

$$\to \eta^* \int \left(\phi(\mathbf{w}^T \mathbf{x}') \phi(\mathbf{w}^T \mathbf{x}) + |a|^2 \phi'(\mathbf{w}^T \mathbf{x}') \phi'(\mathbf{w}^T \mathbf{x}) \mathbf{x}'^{,T} \mathbf{x} \right) \, d\mu_{\infty,t}(da, d\mathbf{w}).$$

It converges, but evolves with time.

A mean-field limit for multi-layered nets?

- Not obvious, how to express a finite-width dynamics in terms of the measure.
- Still, a limit dynamics can be expressed as a measure evolution [Araújo et al., 2019].
- Heuristic: if $\phi(0) = 0$ and initialization is zero-centered, then a limit model vanishes if the number of hidden layers is at least three [Golikov, 2020b].

Open questions:

- Non-asymptotic convergence guarantees, as for the NTK limit?
- Generalization guarantees?

A general treatment

Consider a network with a single hidden layer:

$$f_d(\mathbf{x}) = \sigma(d) \sum_{r=1}^{d} a_r \phi(\mathbf{w}_r^T \mathbf{x}), \quad a_{r;0} \sim \mathcal{N}(0,1),\ \mathbf{w}_{r;0} \sim \mathcal{N}(0,I) \quad \forall r \in [d].$$

- A scaling $\sigma \propto d^{-1/2}$, $\eta = \mathrm{const}$ leads to the **NTK limit** as $d \to \infty$.
- A scaling $\sigma \propto d^{-1}$, $\eta \propto d$ leads to the **mean-field limit** as $d \to \infty$.

Questions:

1. What is a limit dynamics for the default parameterization?
2. Do other hyperparameter scalings lead to "well-defined" limits?
3. Which limit dynamics describe the finite-width one best?

Setup (following [Golikov, 2020a]):

- **A model:**

$$f(\mathbf{x}; W, \mathbf{a}) = \sum_{r=1}^{d} a_r \phi(\mathbf{w}_r^T \mathbf{x}),$$

where ϕ is real analytic.

- **A training procedure**:

$$a_r^{(k+1)} = a_r^{(k)} - \eta_a \mathbb{E}_{\mathbf{x},y} \left(\nabla_{f_d}^{(k)} \ell(\mathbf{x}, y) \phi(\mathbf{w}_r^{(k),T} \mathbf{x}) \right),$$

$$\mathbf{w}_r^{(k+1)} = \mathbf{w}_r^{(k)} - \eta_w \mathbb{E}_{\mathbf{x},y} \left(\nabla_{f_d}^{(k)} \ell(\mathbf{x}, y) a_r^{(k)} \phi'(\mathbf{w}_r^{(k),T} \mathbf{x}) \mathbf{x} \right),$$

$$a_r^{(0)} \sim \mathcal{N}(0, \sigma_a^2), \quad \mathbf{w}_r^{(0)} \sim \mathcal{N}(0, \sigma_w^2 I), \quad \forall r \in [d],$$

where $\nabla_{f_d}^{(k)} \ell(\mathbf{x}, y) = \left. \frac{\partial \ell(y,z)}{\partial z} \right|_{z = f(W^{(k)}, \mathbf{a}^{(k)}, \mathbf{x})}$.

Introduce scaled quantities:

$$\hat{\mathbf{w}}_r = \frac{\mathbf{w}_r}{\sigma_w}, \quad \hat{a}_r = \frac{a_r}{\sigma_a}, \quad \hat{\eta}_w = \frac{\eta_w}{\sigma_w^2}, \quad \hat{\eta}_a = \frac{\eta_a}{\sigma_a^2}.$$

The model becomes:

$$f_d^{(k)}(\mathbf{x}) = \sigma_a \sum_{r=1}^{d} \hat{a}_r^{(k)} \phi(\sigma_w \hat{\mathbf{w}}_r^{(k),T} \mathbf{x}) = \sigma \sum_{r=1}^{d} \hat{a}_r^{(k)} \phi(\hat{\mathbf{w}}_r^{(k),T} \mathbf{x}),$$

where $\sigma = \sigma_a$ and take $\sigma_w = 1$ w.l.o.g.

The training procedure becomes:

$$\hat{\mathbf{w}}_r^{(k+1)} = \hat{\mathbf{w}}_r^{(k)} - \hat{\eta}_w \sigma \mathbb{E}_{\mathbf{x},y} \left(\nabla_{f_d}^{(k)} \ell(\mathbf{x}, y) \hat{a}_r^{(k)} \phi'(\hat{\mathbf{w}}_r^{(k),T} \mathbf{x}) \mathbf{x} \right),$$

$$\hat{a}_r^{(k+1)} = \hat{a}_r^{(k)} - \hat{\eta}_a \sigma \mathbb{E}_{\mathbf{x},y} \left(\nabla_{f_d}^{(k)} \ell(\mathbf{x}, y) \phi(\hat{\mathbf{w}}_r^{(k),T} \mathbf{x}) \right),$$

$$\hat{a}_r^{(0)} \sim \mathcal{N}(0,1) \quad \hat{\mathbf{w}}_r^{(0)} \sim \mathcal{N}(0, I), \quad \forall r \in [d].$$

This dynamics is driven by three hyperparameters: σ, $\hat{\eta}_a$, $\hat{\eta}_w$.

Assume power-law dependencies with respect to width d:

$$\sigma = \sigma^* (d/d^*)^{q_\sigma}, \quad \hat{\eta}_a = \hat{\eta}_a^* (d/d^*)^{\tilde{q}_a}, \quad \hat{\eta}_w = \hat{\eta}_w^* (d/d^*)^{\tilde{q}_w}.$$

$$\sigma = \sigma^* (d/d^*)^{q_\sigma}, \quad \hat{\eta}_a = \hat{\eta}_a^* (d/d^*)^{\tilde{q}_a}, \quad \hat{\eta}_w = \hat{\eta}_w^* (d/d^*)^{\tilde{q}_w}.$$

Available scalings:

1. **NTK:** $q_\sigma = -\frac{1}{2}$, $\tilde{q}_a = \tilde{q}_w = 0$.
2. **Mean-field:** $q_\sigma = -1$, $\tilde{q}_a = \tilde{q}_w = 1$.
3. **"Default":**
   - He initialization: $\sigma = \sigma_a \propto d^{-1/2}$.
   - Constant learning rates: $\eta_a \propto 1 \Rightarrow \hat{\eta}_a = \eta_a \sigma_a^{-2} \propto d$, $\hat{\eta}_w = \eta_w \propto 1$.

   Hence $q_\sigma = -\frac{1}{2}$, $\tilde{q}_a = 1$, $\tilde{q}_w = 0$.
4. **"Sym-default":** $q_\sigma = -\frac{1}{2}$, $\tilde{q}_a = \tilde{q}_w = \frac{1}{2}$. Almost the same dynamics as for the default scaling but $\tilde{q}_a = \tilde{q}_w$.

Assume $\tilde{q}_a = \tilde{q}_w = \tilde{q}$.

Question: can we have a "well-defined" limit model evolution for other scalings?

What do we mean by "well-defined" by the way?

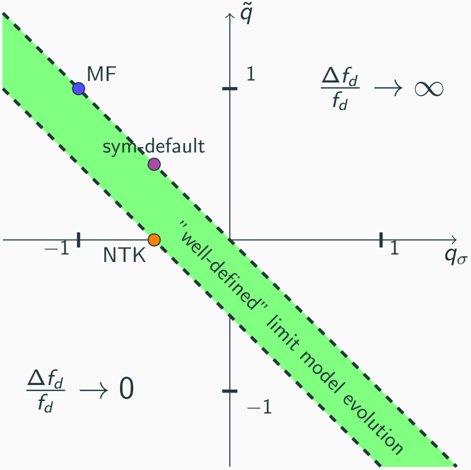
Definition (well-definiteness; informal)
We say "a scaling $(q_\sigma, \tilde{q})$ defines a well-defined limit model" if

$$\exists k^* : \; \forall k \geq k^* \quad \frac{\Delta f_d^{(k)}}{f_d^{(k^*)}} = \Theta_{d \to \infty}(1).$$

Here $\Delta f_d^{(k)} = f_d^{(k+1)} - f_d^{(k)}$.

In other words, the change of logits should be comparable to logits themselves.

Can we have a "well-defined" limit model evolution for other scalings?



Note: MF, NTK, and sym-default scalings are special (later).

Possible properties of limit models:

1. A limit model at initialization is finite;
2. Tangent kernels at initialization are finite;
3. Tangent kernels and a limit model are of the same order at initialization;
4. Tangent kernels start to evolve.

Note: a finite-width model satisfies all of these properties.

Consequence: these properties are necessary for a limit model to approximate a finite-width net.

Each property can be expressed in terms of a scaling:

1. A limit model at initialization is finite:

$$f_d^{(0)} = \Theta_{d\to\infty}(1) \;\Rightarrow\; q_\sigma + 1/2 = 0;$$

2. Tangent kernels at initialization are finite:

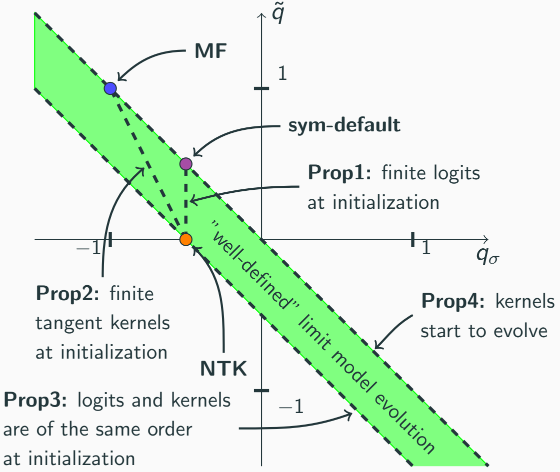
$$K_d^{(0)} = \Theta_{d\to\infty}(1) \;\Rightarrow\; 2q_\sigma + \tilde{q} + 1 = 0;$$

3. Tangent kernels and a limit model are of the same order at initialization:

$$K_d^{(0)} = \Theta_{d\to\infty}(f_d^{(0)}) \;\Rightarrow\; q_\sigma + \tilde{q} + 1/2 = 0;$$

4. Tangent kernels start to evolve:

$$\Delta K_d^{(0)} = \Theta_{d\to\infty}(K_d^{(0)}) \;\Rightarrow\; q_\sigma + \tilde{q} = 0.$$



- NTK, MF, and sym-default limits satisfy the maximal number of properties of finite-width models.
- Each region in the $(q_\sigma, \tilde{q})$-plane corresponds to a distinct limit model. Hence **the number of possible limit models are finite.**

How to satisfy all of these properties in the limit?

Start with a MF-scaling:

$$f_{mf,d}(\mathbf{x}) = \sigma^*(d/d^*)^{-1} \sum_{r=1}^{d} \hat{a}_r \phi(\hat{\mathbf{w}}_r^T \mathbf{x}).$$

It violates property 1: $f_d^{(0)} \to 0$ as $d \to \infty$.

Modify a model:

$$f_{icmf,d}(\mathbf{x}) = \sigma^*(d/d^*)^{-1} \sum_{r=1}^{d} \hat{a}_r \phi(\hat{\mathbf{w}}_r^T \mathbf{x}) + \sigma^*(d/d^*)^{-1/2} \sum_{r=1}^{d} \hat{a}_r^{(0)} \phi(\hat{\mathbf{w}}_r^{(0),T} \mathbf{x}).$$

We call the corresponding limit model an **initialization-corrected mean-field** limit (IC-MF).

Important: IC-MF limit satisfies all of the properties considered above.

Hypothesis: the IC-MF limit approximates the finite-width model better than other limit models.

How to test it?

Consider a "reference" network of width d^*. Assume:

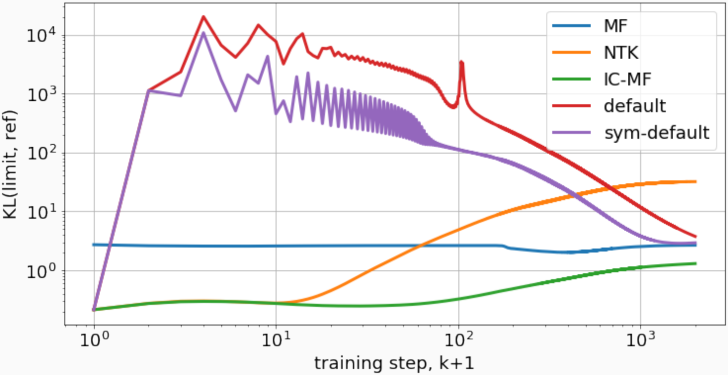
$$\sigma(d) = \sigma^*(d/d^*)^{q_\sigma}, \quad \hat{\eta}_{a/w}(d) = \hat{\eta}^*_{a/w}(d/d^*)^{\tilde{q}_{a/w}}.$$

Consider a metric: $\mathbb{E}_{\mathbf{x}\sim\mathcal{D}} D_{logits}(f_\infty^{(k)}(\mathbf{x}) \,||\, f_{d^*}^{(k)}(\mathbf{x}))$, where

$$D_{logits}(\xi \,||\, \xi^*) = \mathrm{KL}(\mathcal{N}(\mathbb{E}\,\xi, \mathbb{V}\mathrm{ar}\,\xi) \,||\, \mathcal{N}(\mathbb{E}\,\xi^*, \mathbb{V}\mathrm{ar}\,\xi^*)).$$

We measure: $\mathbb{E}_{\mathbf{x}\sim\mathcal{D}} D_{logits}(f_\infty^{(k)}(\mathbf{x}) \,||\, f_{d^*}^{(k)}(\mathbf{x}))$, where

$$D_{logits}(\xi \,||\, \xi^*) = \mathrm{KL}(\mathcal{N}(\mathbb{E}\,\xi, \mathbb{V}\mathrm{ar}\,\xi) \,||\, \mathcal{N}(\mathbb{E}\,\xi^*, \mathbb{V}\mathrm{ar}\,\xi^*)).$$



How do limit dynamics look like:

- **NTK limit:** dynamics in a function space driven by a constant deterministic kernel;
- **MF limit:** deterministic dynamics in a measure space;
- **Sym-default limit:** deterministic dynamics in a measure space too [Golikov, 2020a];
- **Default limit:** again, deterministic dynamics in a measure space.

Take-aways:

1. One can consider an infinite-width limit as a proxy-model for a finite-width net;
2. There are good optimization and generalization guarantees for the NTK limit;
3. The NTK can be computed exactly for simple deep nets;
4. Mean-field and NTK limits are not the only possible ones;
5. There are a finite number of possible infinite-width limits depending on parameter scaling;
6. The NTK limit is not a perfect proxy for finite-width nets;
7. For shallow nets the IC-MF limit is a better proxy than the NTK one.

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