Neural Tangent Kernel: Convergence and Generalization in Neural Networks[1]

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[1]Arthur Jacot, Franck Gabriel, and Clément Hongler. *Neural Tangent Kernel: Convergence and Generalization in Neural Networks*. Feb. 10, 2020. arXiv: 1806.07572 [cs, math, stat]. URL: http://arxiv.org/abs/1806.07572 (visited on 08/13/2023). preprint.

On the equivalence of Neural Network and Kernel Machine

On the equivalence at initialization—Infinity width Multi-Layer Perceptron (MLP) initialize with Gaussian weights and biases is equivalent to a Gaussian Process.[2]

On the equivalence at training—Infinity width MLP with ReLU activation under squared loss trained by gradient descent is equivalent to a Gaussian Process.[3]

On the equivalence at training—Infinite width MLP with ReLU activation under soft margin loss trained by subgradient descent is equivalent to a support vector machine.[4]

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[2] Jaehoon Lee et al. *Deep Neural Networks as Gaussian Processes*. Mar. 2, 2018. arXiv: `1711.00165 [cs, stat]`. URL: `http://arxiv.org/abs/1711.00165` (visited on 07/08/2023). preprint.

[3] Jacot, Gabriel, and Hongler, *Neural Tangent Kernel*.

[4] Yilan Chen et al. *On the Equivalence between Neural Network and Support Vector Machine*. Nov. 11, 2021. arXiv: `2111.06063 [cs, math, stat]`. URL: `http://arxiv.org/abs/2111.06063` (visited on 05/27/2022). preprint.

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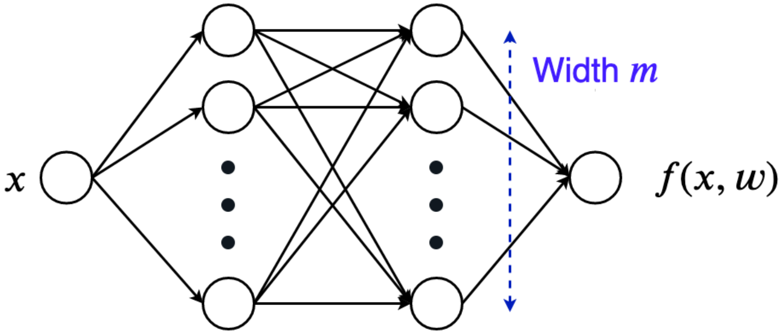
The Architecture of a Multi-Layer Perceptron (MLP)



Notations—Parameters Space

L: the depth of the network (*a.k.a.* the number of layers). *E.g.* 0 is the input layer, L is the output layer.

$N^{(L)}$: the width of the network (*a.k.a.* the number of neurons in each layer). *E.g.* $N^{(0)}$ is the dimension of the input, $N^{(L)}$ is the dimension of the output.

P: the total number of parameters, which is $\sum_{l=1}^{L} N^{(l-1)} N^{(l)}$.

The parameters between each layer are denoted as $W^{(l)} \in \mathbb{R}^{N^{(l-1)} \times N^{(l)}}$ and $b^{(l)} \in \mathbb{R}^{N^{(l)}}$, which are initialized as i.i.d. N$(0, 1)$.

Notations—Function Space

σ: the activation function. *E.g.* $\sigma(x) = \max\{0, x\}$ is the ReLU.

$\mathcal{F}$: the function space of the MLP. *E.g.* $\mathcal{F} = \{f : \mathbb{R}^{N^{(0)}} \to \mathbb{R}^{N^{(L)}}\}$.

$\tilde{f}_\theta^{(l)}(x) : \mathbb{R}^{(l-1)} \to \mathbb{R}^{(l)}$: the pre-activations

$f_\theta^{(l)}(x) : \mathbb{R}^{(l)} \to \mathbb{R}^{(l)}$: the post-activations

Clearly, we have $\theta \in \mathbb{R}^P$ and

$$
\begin{aligned}
f_\theta^{(0)}(\mathbf{x}) &= \mathbf{x} \\
\tilde{f}_\theta^{(l)}(\mathbf{x}) &= W^{(l)\mathsf{T}} f_\theta^{(l-1)}(\mathbf{x}) + b^{(l)} \\
f_\theta^{(l)}(\mathbf{x}) &= \sigma(\tilde{f}_\theta^{(l)}(\mathbf{x}))
\end{aligned}
$$

Gradient Descent—Parameter Space

For a task with input $x \in \mathbb{R}^{n \times N^{(0)}}$ and output $y \in \mathbb{R}^{n \times N^{(L)}}$, the total loss $\mathcal{L}$ is defined with per-sample loss ℓ

$$\mathcal{L}(\theta) = \underset{\theta}{\text{argmin}} \frac{1}{n} \sum_{i=1}^{n} \ell(\mathcal{F}(\mathbf{x}_i), y_i).$$

According to the chain rule, the gradient of the loss is

$$\nabla_\theta \mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \nabla_\theta \mathcal{F}(\mathbf{x}_i) \nabla_{\mathcal{F}} \ell(\mathcal{F}, y_i).$$

If we let the gradient descent update the parameters with infinitisimal step size, then the gradient descent can be approximated as a derivative on the time dimension t

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = -\nabla_\theta \mathcal{L}(\theta) = -\frac{1}{n} \sum_{i=1}^{n} \nabla_\theta \mathcal{F}(\mathbf{x}_i) \nabla_{\mathcal{F}} \ell(\mathcal{F}, y_i).$$

Gradient Descent—Function Space

Then for any pair $(\mathbf{x}^*, \mathbf{x}_i)$, the output of the network slowly evolves as

$$\frac{\mathrm{d}\mathcal{F}(\mathbf{x}^*)}{\mathrm{d}t} = \frac{\mathrm{d}\mathcal{F}(\mathbf{x}^*)}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}t} = -\frac{1}{n}\sum_{i=1}^{n} \nabla_\theta \mathcal{F}(\mathbf{x}^*)^\mathsf{T} \nabla_\theta \mathcal{F}(\mathbf{x}_i) \nabla_{\mathcal{F}} \ell(\mathcal{F}, y_i).$$

And the inner product of the gradient defines the Neural Tangent Kernel (NTK), which is also called kernel gradient

$$K(\mathbf{x}^*, x_i) = \nabla_\theta \mathcal{F}(\mathbf{x}^*)^\mathsf{T} \nabla_\theta \mathcal{F}(\mathbf{x}_i)$$

With random features[5] of p (where $p \ll P$) samples of function space $\mathcal{F}_k^p$, these functions define a linear parametrization: $\mathbb{R}^P \rightarrow \mathcal{F}$ and the NTK can be approximated as

$$K(\mathbf{x}^*, \mathbf{x}_i) \approx \mathbb{E}\left[f_k^p(\mathbf{x}^*)^\mathsf{T} f_k^p(\mathbf{x}_i)\right].$$

[5] Ali Rahimi and Benjamin Recht. “Random Features for Large-Scale Kernel Machines”. In: ().

The good and the bad

Recall the knowledge of Convex Optimization, the gradient descent converges to the global minimum of the convex loss function. For NTK,

The Good: For the MLP trained by gradient descent, the network output slowly evolves along the (negative) kernel gradient with respect to the neural tangent kernel (NTK) during training.

The Bad: The MLP (not to mention other NN architectures) is usually non-convex and the linear parametrization does not exist. Which leads to unstable NTK at initialization and during training.

Question: Can we prove the NTK is deterministic and staying constant, for example in an asymptotic manner?

NTK becomes deterministic at initialization[6]

Theorem: Neural Network as Gaussian Process

For a network of depth L at initialization, with a Lipschitz nonlinearity σ, and in the limit as the layers width $n_1, n_2, \ldots, n_L \to \infty$, the NTK $\Theta^{(L)}$ converges in probability to a deterministic limiting kernel:

$$\Theta^{(L)} \to \Theta_\infty^{(L)} \otimes I_{N_L}.$$

The scalar kernel $\Theta_\infty^{(L)} : \mathbb{R}^{N_0} \times \mathbb{R}^{N_0} \to \mathbb{R}$ is defined recursively as

$$\begin{aligned}
\Theta_\infty^{(1)}(\mathbf{x}^*, \mathbf{x}_i) &= \Sigma_\infty^{(1)}(\mathbf{x}^*, \mathbf{x}_i) \\
\Theta_\infty^{(L+1)}(\mathbf{x}^*, \mathbf{x}_i) &= \Theta_\infty^{(L+1)}(\mathbf{x}^*, \mathbf{x}_i)\dot{\Sigma}_\infty^{(L+1)}(\mathbf{x}^*, \mathbf{x}_i) + \Sigma_\infty^{(L+1)}(\mathbf{x}^*, \mathbf{x}_i) \\
\dot{\Sigma}_\infty^{(L+1)}(\mathbf{x}^*, \mathbf{x}_i) &= \mathbb{E}_{f\sim \mathsf{N}(0,\Sigma^{(L)})}[\dot{\sigma}(f(\mathbf{x}^*))\dot{\sigma}(f(\mathbf{x}_i))]
\end{aligned}$$

[6] Lee et al., *Deep Neural Networks as Gaussian Processes*.

The NTK is constant during training

Previously, we have shown that (omit the inputs for simplicity)

$$\frac{\mathrm{d}\mathcal{F}_\theta}{\mathrm{d}t} = -\alpha \mathbf{K}_\infty \nabla_f \mathcal{L}.$$

To track the evolution of θ in time, we can consider it as a function of time t. With Taylor expansion, we have[7]

$$\begin{aligned}
\mathcal{F}_\theta(t) &= \mathcal{F}_\theta(0) + \nabla_\theta \mathcal{F}_\theta(0)[\theta(t) - \theta(0)] \\
\theta(t) - \theta(0) &= -\alpha \nabla_\theta \mathcal{F}_\theta^{\mathsf{T}} \nabla_f \mathcal{L} \\
\mathcal{F}_\theta(t) - \mathcal{F}_\theta(0) &= -\alpha \nabla_\theta \mathcal{F}_\theta(0)^{\mathsf{T}} \nabla_\theta \mathcal{F}(\mathbf{X}; \theta(0)) \nabla_f \mathcal{L} \\
\frac{\mathrm{d}\mathcal{F}_\theta(t)}{\mathrm{d}t} &= -\alpha K(\theta(0)) \nabla_f \mathcal{L} \\
&= -\alpha \mathbf{K}_\infty \nabla_f \mathcal{L}
\end{aligned}$$

[7] Jaehoon Lee et al. "Wide Neural Networks of Any Depth Evolve as Linear Models Under Gradient Descent". In: *Journal of Statistical Mechanics: Theory and Experiment* 2020.12 (Dec. 1, 2020), p. 124002. ISSN: 1742-5468. DOI: 10.1088/1742-5468/abc62b. arXiv: 1902.06720 [cs, stat]. URL: http://arxiv.org/abs/1902.06720 (visited on 08/13/2023).

The light that is Shed by the NTK

- With the equivalence of the NTK and the Gaussian Process, Bayesian Inference can be applied to explain the generalization of the neural network.
- For the same reason, the computation technique of Bayesian Inference (*e.g.* MCMC) can be applied to the neural network.
- Since NTK is the gradient defined on the function space, calculus of variations can be applied to the neural network.
- Other analytic tools such as Spectrum Analysis or Random Matrix can be applied to find tighter bounds.

The Undiscovered Area

- Empirical results shows that the Neural Network optimized by NTK does not achieve State-of-the-Art (SOTA) performance.
- The condition of the equivalence of NTK and Gaussian Process is too strong, which might not be practical.
- The NTK of other architectures (*e.g.* CNN, RNN) is not well studied (Has been majorly solved in 2023).