Neural Tangent Kernel

Insights from High-Dimensional Probability

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December 20, 2024

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NTK

The **Neural Tangent Kernel (NTK)** captures the behavior of fully-connected deep nets in the infinite-width limit trained by gradient descent. [Jacot et al., 2018]

- An attraction is that a pure kernel-based method is used to capture the power of a fully-trained deep net of infinite width.
- NTK explains the evolution of neural networks during gradient descent training.
- Insight into why wide neural networks can consistently converge to a global minimum when minimizing empirical loss.

Derivation

- Model Parameters $\theta \in \mathbb{R}^P$
- The empirical loss function $\mathscr{L} : \mathbb{R}^P \to \mathbb{R}_+$ to minimize during training is defined as follows, using a per-sample cost function $\ell : \mathbb{R}^{n_0} \times \mathbb{R}^{n_L} \to \mathbb{R}_+$

$$\mathscr{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \ell(f(\mathbf{x}^{(i)}; \theta), y^{(i)})$$

- According to the chain rule. the gradient of the loss is:

$$\nabla_\theta \mathscr{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \underbrace{\nabla_\theta f(\mathbf{x}^{(i)}; \theta)}_{\text{size } P \times n_L} \underbrace{\nabla_f \ell(f, y^{(i)})}_{\text{size } n_L \times 1}$$

Derivation

- Each gradient descent update introduces a small incremental change of an infinitesimal step size

$$\frac{d\theta}{dt} = -\nabla_\theta \mathscr{L}(\theta) = -\frac{1}{N}\sum_{i=1}^{N} \nabla_\theta f(\mathbf{x}^{(i)};\theta)\nabla_f \ell(f, y^{(i)})$$

- Again, by the chain rule, the network output evolves according to the derivative:

$$\frac{df(\mathbf{x};\theta)}{dt} = \frac{df(\mathbf{x};\theta)}{d\theta}\frac{d\theta}{dt} = -\frac{1}{N}\sum_{i=1}^{N} \underbrace{\nabla_\theta f(\mathbf{x};\theta)^\top \nabla_\theta f(\mathbf{x}^{(i)};\theta)}_{\text{Neural tangent kernel}} \nabla_f \ell(f, y^{(i)})$$

Derivation

- Here we find the Neural Tangent Kernel (NTK), as defined in the blue part in the last formula: $K : \mathbb{R}^{n_0} \times \mathbb{R}^{n_0} \to \mathbb{R}^{n_L \times n_L}$

$$K(\mathbf{x}, \mathbf{x}'; \theta) = \nabla_\theta f(\mathbf{x}; \theta)^\top \nabla_\theta f(\mathbf{x}'; \theta)$$

- Each entry:

$$K_{m,n}(\mathbf{x}, \mathbf{x}'; \theta) = \sum_{p=1}^{P} \frac{\partial f_m(\mathbf{x}; \theta)}{\partial \theta_p} \frac{\partial f_n(\mathbf{x}'; \theta)}{\partial \theta_p}$$

- The feature map form of one input: $\varphi(\mathbf{x}) = \nabla_\theta f(\mathbf{x}; \theta)$

NTK First Results

- Most critical proposition from the NTK paper
- When $n_1, \ldots, n_L \to \infty$ (network with infinite width), the NTK converges to be:
  1. Kernel is irrelevant to the initialization values
  2. Kernel stays constant during training.

Problem Definition

A single hidden-layer neural network with i.i.d. random parameters, in the limit of infinite width, is a function drawn from a Gaussian process (GP) [Neal, 1996].

$$\Sigma^{(1)}(\mathbf{x}, \mathbf{x}') = \frac{1}{n_0}\mathbf{x}^\top \mathbf{x}' + \beta^2$$

$$\Lambda^{(l+1)}(\mathbf{x}, \mathbf{x}') = \begin{bmatrix} \Sigma^{(l)}(\mathbf{x}, \mathbf{x}) & \Sigma^{(l)}(\mathbf{x}, \mathbf{x}') \\ \Sigma^{(l)}(\mathbf{x}', \mathbf{x}) & \Sigma^{(l)}(\mathbf{x}', \mathbf{x}') \end{bmatrix}$$

$$\Sigma^{(l+1)}(\mathbf{x}, \mathbf{x}') = \mathbb{E}_{f \sim \mathcal{N}(0, \Lambda^{(l)})}[\sigma(f(\mathbf{x}))\sigma(f(\mathbf{x}'))] + \beta^2$$

- To give the formula of NTK with this GP, we also need to define a derivative covariance:

$$\dot{\Sigma}^{(h)}(x, x') = c_\sigma \mathbb{E}_{(u,v)\sim\mathcal{N}(0,\Lambda^{(h)})}\left[\dot{\sigma}(u)\dot{\sigma}(v)\right].$$

- The final NTK expression for the fully-connected neural network is

$$\Theta^{(L)}(x, x') = \sum_{h=1}^{L+1}\left(\Sigma^{(h-1)}(x, x') \cdot \prod_{h'=h}^{L+1}\dot{\Sigma}^{(h')}(x, x')\right),$$

where $\Sigma^{(h-1)}(x, x')$ and $\dot{\Sigma}^{(h')}(x, x')$ are layer-specific covariance and derivative covariance terms.

Problem Definition

(The original paper has an asymptotic expression but this is later proven)

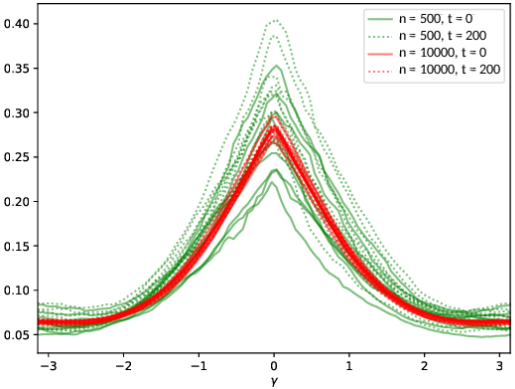
Theorem (Convergence to the NTK at initialization). Fix $\epsilon > 0$ and $\delta \in (0,1)$. Suppose

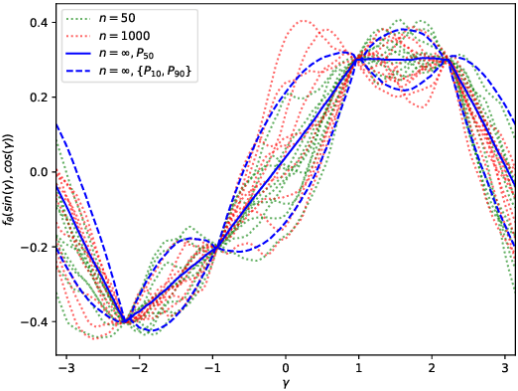
$$\sigma(z) = \max(0,z) \quad \text{and} \quad \min_{h \in [L]} d_h \geq \Omega\left(\frac{L^6}{\epsilon^4} \log\left(\frac{L}{\delta}\right)\right).$$

Then for any inputs $x, x' \in \mathbb{R}^{d_0}$ such that $\|x\| \leq 1, \|x'\| \leq 1$, with probability at least $1-\delta$, we have:

$$\left| \left\langle \frac{\partial f(\theta, x)}{\partial \theta}, \frac{\partial f(\theta, x')}{\partial \theta} \right\rangle - \Theta^{(L)}(x, x') \right| \leq (L+1)\epsilon.$$

Experiments





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CNTK

- The first efficient exact algorithm for computing the extension of NTK to convolutional neural nets, which we call Convolutional NTK
- Theoretically, also gives the first non-asymptotic proof showing that a fully-trained sufficiently wide net is indeed equivalent to the kernel regression predictor using NTK.

Finite Width and Spectral Bias

- Found some results on finite-width case
- consequently, eigenfunctions of the NTK integral operator are learned at rates corresponding to their eigenvalues

Generalization Bound

- Assuming:
- Fix failure probability $\delta \in (0,1)$
- data $S = \{(x_i, y_i)\}_{i=1}^{n}$
- Distribution D is $(\lambda_0, \delta/3, n)$-non-degenerate.
- $\kappa = \mathcal{O}\left(\frac{\lambda_0 \delta}{n}\right)$.
- Width $m \geq \kappa^{-2}\text{poly}(n, \lambda_0^{-1}, \delta^{-1})$.
- Loss function $\ell : \mathbb{R} \times \mathbb{R} \to [0,1]$ is 1-Lipschitz in the first argument such that $\ell(y,y) = 0$.
- Gradient descent runs for $k \geq \Omega\left(\frac{1}{\eta\lambda_0} \log \frac{n}{\delta}\right)$ iterations.

Generalization Bound

- Then with probability at least $1-\delta$ over the random initialization and the training samples,The two-layer neural network $f_{\mathbf{W}(k),\mathbf{a}}$ has population loss $L_D(f_{\mathbf{W}(k),\mathbf{a}}) = \mathbb{E}_{(\mathbf{x},y)\sim D}[\ell(f_{\mathbf{W}(k),\mathbf{a}}(\mathbf{x}), y)]$, bounded as:

$$L_D(f_{\mathbf{W}(k),\mathbf{a}}) \leq \sqrt{\frac{2\mathbf{y}^\top (\mathbf{H}^\infty)^{-1}\mathbf{y}}{n}} + O\left(\sqrt{\frac{\log \frac{n}{\lambda_0 \delta}}{n}}\right).$$

Uniform Convergence

- Overparametrized Multilayer Neural Networks: Uniform Concentration of Neural Tangent Kernel and Convergence of Stochastic Gradient Descent (2024)
- They first show that with random initialization, the NTK function converges to some deterministic function **uniformly** in input for all layers as the number of neurons tends to infinity
- Then they apply the uniform convergence result to further prove that the prediction error of multi-layer neural networks under SGD converges in expectation in the streaming data setting

Uniform Convergence

Theorem Under Gaussian initialization, for $m \geq Cd^2 \exp(L^2)$ for some constant C, there exist constants C_1, C_2, and C_3 such that, with probability at least $1 - \exp(-C_1 m^{1/3})$,

$$\left\| H^{(\ell)} - \Phi^{(\ell)} \right\|_\infty \leq C_2 \left(\frac{C_3^L}{m^{1/6}} + \sqrt{\frac{dL \log m}{m}} \right), \quad \forall 1 \leq \ell \leq L.$$

Sensitivity Analysis

- **Sensitivity Definition:**

$$\mathcal{S}_{f_\theta}(z) = \mathbb{E}_{z,\hat{z},\theta}|\nabla_z f(z,\theta)^\top (z-\hat{z})|$$

- **NTK Sensitivity:**

$$\mathcal{S}_{NTK}(z) = \|z\|_2 \|\nabla_z \Phi_{NTK}(z)^\top \Phi_{NTK}^\top K_{NTK}^{-1} Y\|_2$$

Which results in:

$$\mathcal{S}_{NTK}(z) = \mathcal{O}\left(logk\sqrt{\frac{ND}{p}}\right) \sim \mathcal{O}(1)$$

Future Research Directions

- **Relax Assumptions:**
  - **High-dimensional regime:**

$$Nlog^3 N\wr(d^{\frac{3}{2}})$$

    It's an open question whether this can be relaxed or not.
  - **Data distibution:** P_X satisfies the *Lipschitz concentration property*. Namely, there exists an absolute constant $c > 0$ such that, for every Lipschitz continuous function $\varphi : \mathbb{R}^d \to \mathbb{R}$, we have for all $t > 0$,

$$\mathbb{P}\left(\left|\varphi(x) - \mathbb{E}_X[\varphi(x)]\right| > t\right) \leq 2e^{-ct^2/\|\varphi\|^2_{\text{Lip}}}$$

    Some distributions that satisfy this property include the Gaussian distribution and the uniform distribution, or data obtianed be GANs.
  - **Even Activation Functions:** Even activation functions are used to prove the upper bound of the NTK by Bombari et al. (2022).

Spurious Data Memorization

- **Spurious Data :**
  - **Definition:** Spurious data is data that is not relevant to the task at hand, but is still memorized by the model.
  - **Formulation:**

$$z_i = \begin{bmatrix} x_i \\ y_i \end{bmatrix} \quad \text{and} \quad z_i^s = \begin{bmatrix} x \\ y_i \end{bmatrix}$$

where x is independent of x_i.

- **Future Alignment:**

$$\mathscr{F}_\varphi(z, z_1) := \frac{\varphi(z)^\top P^\perp_{\Phi_{-1}} \varphi(z_1)}{\left\| P^\perp_{\Phi_{-1}} \varphi(z_1) \right\|_2^2}$$

- **Satbiblity:**

$$S_{z_1}(z) = \mathscr{F}_\varphi(z, z_1) S_{z_1}(z_1)$$

Memorization in NTK Feutures

$$\left|\mathscr{F}_{\mathrm{NTK}}(z_1^s, z_1) - \gamma_{\mathrm{NTK}}\right| = o(1),$$

where

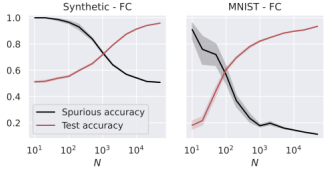
$$0 < \gamma_{\mathrm{NTK}} := \alpha \frac{\sum_{l=1}^{+\infty} \mu_l'^2 \alpha^l}{\sum_{l=1}^{+\infty} \mu_l'^2} < 1, \tag{26}$$

and μ_l' is the l-th Hermite coefficient of the derivative of the activation φ'.
The generalization of the NTK is given by:

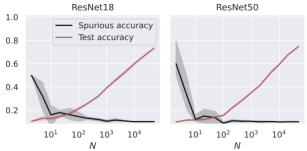
$$\mathrm{Cov}\left(f_{\mathrm{NTK}}(z_1^s, \theta^*), g_1\right) \leq \gamma_{\mathrm{NTK}} \sqrt{\mathscr{R}_{Z_{-1}}} \sqrt{\mathrm{Var}(g_1)}$$

Future Directions

- Fully Connected Neural Networks NTK Generalization and Memorization:



- Convolutional Neural Networks NTK Generalization and Memorization:



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Our Proposal

- Guarantees with other/practical Assumptions
  - NTK-like results on Attention Mechanism
  - Extending current results on Gaussian/Bounded to sub-Gaussian or sub-Exponential
- NTK on Unsupervised settings like Generative modeling or Self-Supervised or Transfer learning
- NTK on other architectures like Kolmogorov Arnold Networks, Transformers etc
- NTK Spectral Distribution
- Optimization methods other than (Stochastic) Gradient Descent. e.g. Momentum SGD, using Long Search for GD.
- Certain activation functions. e.g. tanh
- Random number of neurons in Layers.
- Finding Sample complexity, VC-Dimensions, Rademacher Complexity

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