Neural Tangent Kernel

Comprehending Convergence & Generalization in Neural Networks[1]

J. Setpal

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MACHINE LEARNING
@ PURDUE

[1] Jacot, Gabriel, Hongler. [NIPS 2018]

Outline

1. Background & Intuition

2. Neural Tangent Kernel

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Problem Setting

Given network $f_\theta : \mathbb{R}^d \to \mathbb{R}$, we have two distinctive regimes:

Underparameterized Learning: $\boldsymbol{n \geq p}, \quad \theta \in \mathbb{R}^p, \quad \mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$

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Either way, we optimize θ to minimize an empirical loss (here, quadratic):

$$\mathcal{L}(\theta, \mathcal{D}) = \frac{1}{n} \sum_{i=1}^{n} \ell(f_\theta(x_i), y_i) = \frac{1}{n} \| f_\theta(\boldsymbol{x}) - \boldsymbol{y} \|_2^2 \tag{1}$$

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A: NTK's approach:

a. Construct an analogy to a simpler paradigm (kernel methods).
b. Prove the analogy actually holds for sufficiently wide networks.
c. Use the analysis from the kernel method to understand training dynamics of the neural network.

Pre-Requisite 1/3 – Taylor Series

We can approximate function g using a polynomial via the Taylor Series:

$$P_a(x) = \sum_{i=0}^{\infty} \frac{g^{(n)}(a)}{n!}(x-a)^n \tag{2}$$

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We will use the first-order approximation to model **training dynamics in neural networks**.

Pre-Requisite 2/3 – Operator Norm

The operator norm of matrix A is the maximum amount of stretching that A can do to arbitrary vector x:

$$A \in \mathbb{R}^{m \times n}, \quad x \in \mathbb{R}^n \tag{4}$$

$$\|A\|_{\text{op}} = \max_{x \in \mathbb{R}^n} \frac{\|Ax\|_p}{\|x\|_q} \tag{5}$$

Usually $p = q = 2$.

Pre-Requisite $^3/_3$ – Kernel Methods

$K : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ is a kernel if $\exists \phi : \mathcal{X} \to \mathcal{H}$ s.t:

$$K(x, x') = \phi(x)^T \phi(x') = \langle \phi(x), \phi(x') \rangle \tag{6}$$

Any PSD matrix defines a kernel.

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As an example:

$$\hat{y} = \textbf{sgn} \sum_{i=1}^{n} w_i y_i k(x, x') \tag{7}$$

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Neural Network Setup

We have fully-connected network f_θ with $n_0, \ldots, n_L$ neurons in each layer, activation function $\sigma : \mathbb{R} \to \mathbb{R}$ with pre-activations $\tilde{\alpha}$ and activations α defined recursively as follows:

$$\alpha^{(0)}(x;\ \theta) = x \tag{8}$$

$$\tilde{\alpha}^{(\ell+1)}(x;\ \theta) = \frac{1}{\sqrt{n_\ell}} W^{(\ell)} \alpha^{(\ell)}(x;\theta) + \beta b^{(\ell)} \tag{9}$$

$$\alpha^{(\ell)}(x;\ \theta) = \sigma(\tilde{\alpha}^{(\ell)}(x;\theta)) \tag{10}$$

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Aside

Factors $1/\sqrt{n_\ell}$, β scale gradients & enable consistent aymptotic behavior.

Studying Convergence in Function Space

Notice that quadratic loss[2] is **convex w.r.t. function space** but often **non-convex w.r.t. parameter space**.

$$C : \mathcal{F} \to \mathbb{R} \qquad \text{Convex :D} \tag{11}$$

$$C \circ F^{(L)} : \mathbb{R}^p \to \mathbb{R} \qquad \text{Highly Non-Convex D:} \tag{12}$$

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We'll answer the questions in detail, but in reverse order.

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Lazy Learning

For L-smooth f, gradient descent using small η guarantees convergent loss.

$$\mathcal{L}(\theta_{t+1}, \mathcal{D}) \leq \mathcal{L}(\theta_t, \mathcal{D}), \quad \eta \leq 1/L \tag{13}$$

$$\|\theta - \theta_0\| \approx \frac{\|f_{\theta_0}(x) - y\|}{\|\nabla_\theta f_{\theta_0}(x)\|_{\text{op}}} \tag{14}$$

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Takeaway: With gaussian initialization, as $\theta \in \mathbb{R}^p$ s.t. $p \to \infty$

$$\exists \theta^* \quad \text{s.t.} \quad \mathcal{L}(f_{\theta^*}, \mathcal{D}) = \min_\theta \mathcal{L}(f_\theta, \mathcal{D}) \quad \text{and} \quad \|\theta^* - \theta_0\| < B \ll \infty \tag{15}$$

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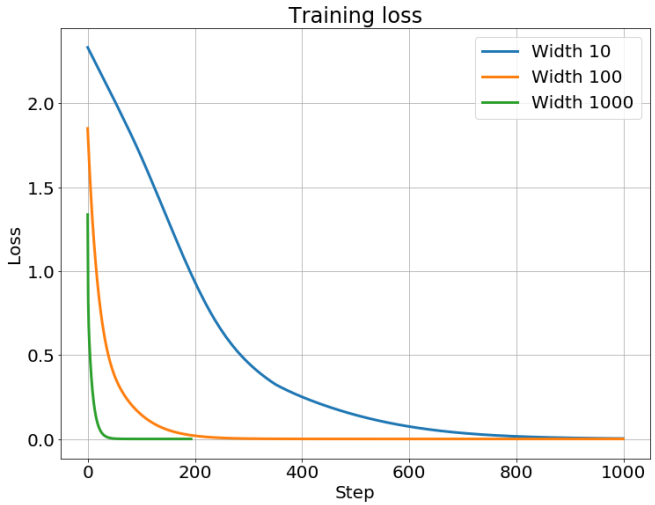
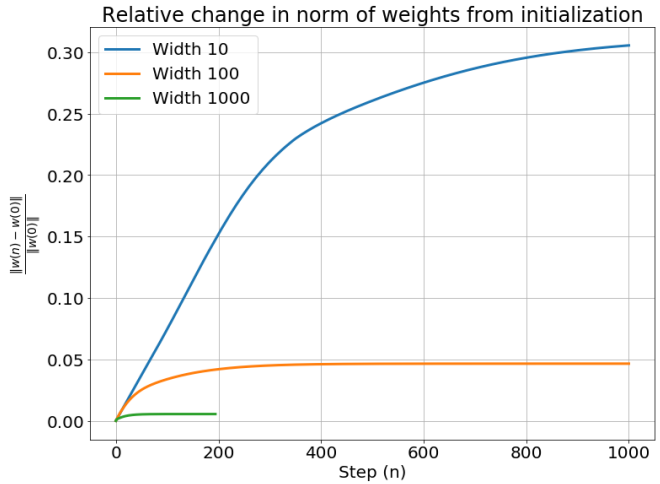
We can see this by the change of $\|\theta\|$ as $\theta \in \mathbb{R}^{10}, \mathbb{R}^{100}, \mathbb{R}^{1000}$:





Linear Approximation of f_θ

Applying first-order taylor expansion of f with respect to the evolution of parameters θ, we have:

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Since we are in the overparameterized lazy learning regime, we have $\theta \approx \theta_0$, and $g_\theta \approx f_\theta$, which means:

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Now for $G^{(L)} : \mathbb{R}^p \to \mathcal{G}$ cost-composition $C \circ G^L : \mathbb{R}^p \to \mathbb{R}$ is convex!!

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We can use this to define feature map Φ over the entire dataset:

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Caveat: We're discussing gradient descent, not *stochastic* gradient descent. In practice, we see performance dropoffs when optimizing over g_θ.

Defining NTK

We can define a kernel using our feature map ϕ:

$$\kappa(x, x') = \phi(x)^T \phi(x') = \langle \nabla_\theta f_{\theta_0}(x), \nabla_\theta f_{\theta_0}(x') \rangle \tag{21}$$

This kernel is the **neural tangent kernel**.

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The NTK effectively exists as part of gradient descent:

$$\theta_{t+1} = \theta_t - \nabla_\theta \mathcal{L}(f_{\theta_t}, \mathcal{D}) \tag{22}$$

$$\frac{\partial \theta}{\partial t} = -\eta \nabla_\theta \mathcal{L}(\theta, \mathcal{D}) = -\frac{\eta}{n} \sum_{i=1}^{n} \nabla_\theta f_\theta(x_i) \nabla_{f_\theta} \ell(f_\theta, y_i) \tag{23}$$

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The NTK depends on θ_0, is random at initialization and varies during training, but in the limit, this changes.

Limiting Behavior of NTK

When the width tends to infinity, the NTK is deterministic at intitialization and doesn't change through training:

$$k \to \infty \implies f_{\theta,k} \to \mathcal{N}(0, \Sigma_k) \; \forall k \in \{1, \ldots, n_L\} \tag{25}$$

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Where covariance matrices Σ_k are defined recursively as follows:

$$\Sigma_1(x, x') = \frac{1}{n_0} x^T x' + \beta^2 \tag{26}$$

$$\Sigma_{k+1}(x, x') = \mathbb{E}_{f \sim \mathcal{N}(0, \Sigma_k)}[\sigma(f(x))\sigma(f(x'))] + \beta^2 \tag{27}$$

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$$\Sigma_{k+1}(x, x') = \mathbb{E}_{f \sim \mathcal{N}(0, \Sigma_k)}[\sigma(f(x))\sigma(f(x'))] + \beta^2 \tag{27}$$

Which we further defines the limiting NTK:

$$\kappa_1(x, x') = \Sigma_1(x, x') \tag{28}$$

$$\kappa_{k+1}(x, x') = \kappa_k(x, x')\Sigma'_{k+1}(x, x') + \Sigma_k(x, x') \tag{29}$$

$$\Sigma'_{k+1}(x, x') = \mathbb{E}_{f \sim \mathcal{N}(0, \Sigma_k)}[\sigma'(f(x))\sigma'(f(x'))] + \beta^2 \tag{30}$$

Which is independent of initialization.

Training within the NTK Regime

During training f_θ follows a descent along the negative kernel gradient:

$$\partial_t f_{\theta_t} = -\nabla_{\Phi_{(L)}} C_{|f_{\theta_t}} \tag{31}$$

The Limiting Kernel is always *positive definite*. By performing an eigendecomposition, we can decouple the gradient flow into eigenvectors, that decay at the rate of their eigenvalues.

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Caveat: Computing NTK is expensive $\Omega(n^2)$ while regular GD uses $\mathcal{O}(d)$ samples.

Thank you!

Have an awesome rest of your day!

Slides: https://jinen.setpal.net/slides/ntk.pdf

References:

1. Dwaraknath, Rajat. (Nov 2019). Understanding the Neural Tangent Kernel. https://www.eigentales.com/NTK/
2. Ma, Tengyu. (Nov 2022). Stanford CS229M - Lecture 13: Neural Tangent Kernel. https://youtu.be/btphvvnad0A
3. Ma, Tengyu. (Nov 2022). Stanford CS229M - Lecture 14: Neural Tangent Kernel, Implicit regularization of gradient descent. https://youtu.be/xpT1ymwCk9w
4. Weng, Lilian. (Sep 2022). Some math behind neural tangent kernel. https://lilianweng.github.io/posts/2022-09-08-ntk/
5. Pietraho, Thomas. Math 2805: Mathematical principles of machine learning. https://web.bowdoin.edu/~tpietrah/hugo/math2805/docs/unsupervised_learning/dim_reduction/hw_operator_norms/