

- Wide . Neural networks as GP
- . The NTK . Deep NN < R class

• Pb know k
Obstrue
$$(x^{1:n}, y^{1:n} = f(x^{1:n})) = \omega$$

Bayesian: Prior $f \sim GP(O, R)$
Restenior $f \mid \omega = ?$

Lecture VII – Wide multilayer networks and the Neural Tangent Kernel (NTK)

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The Neural Tangent Kernel (NTK)

Wide networks and Gaussian Processes

The NTK is constant during training Example – regression and \mathcal{L}_{LS}

Wide and deep networks and classification

Notation

- Neural network predictor $f(x; \theta)$, where $x \in \mathbb{R}^d$
- For each layer l = 1 : L of dimension m_l , with $x^0 \equiv x$, and $z^L \equiv f(x)$

$$z^{l+1} = W^{l+1}x^{l} + b^{l+1} \qquad x^{l+1} = \phi(z^{l+1})$$
(1)

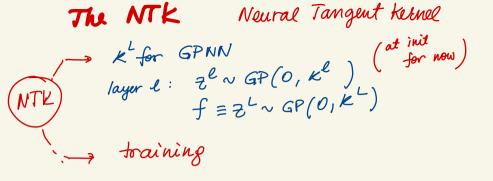
Here $x^{l,l+1}, z^{l+1}, b^{l+1}$ are column vectors W^{l+1} is a $m_{l+1} \times m_l$ matrix, $\phi()$ is the non-linearity/activation function.

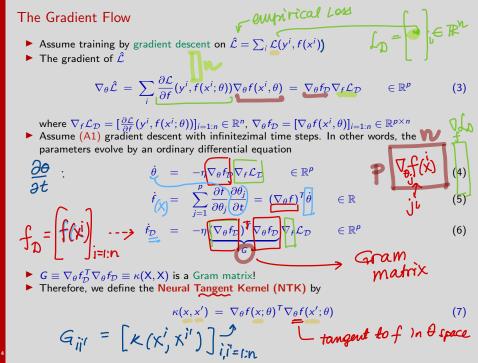
The weights

$$W_{ij}^{\prime} = \sigma_w w_{ij}^{\prime} / \sqrt{m_l}, \qquad b_j^{\prime} = \sigma_b eta_j^{\prime}, \quad$$
Known as NTK parametrization (2)

- ▶ Parameter vector $\theta = \text{vector}\{w^{1:L}, \beta^{1:L}\} \in \mathbb{R}^p$ initialized i.i.d. ~ N(0, 1)
- $\sigma_{w,b}$ are fixed hyper-parameters, $1/\sqrt{m_l}$ normalizes the expected norm of W^l columns • Loss $\mathcal{L}(y, f)$
- We want to analize the behavior of this network f() at initialization and during training, when m_{1:L} very large
- Three approximations help analysis
 - (A1) continuous time training, called gradient flow
 - (A2) $m_{1:L} \to \infty$ in the wide limit, we can apply the Central Limit Theorem (CLT), and Gaussian Processes
 - (A3) parameters θ do not change much during training, i.e. $\theta_t \theta_0$ is small

$$\begin{array}{c} \chi^{e} = \chi \\ \text{input} \\ \mathbb{P}^{e} \mathbb{N} \\ \mathbb{P}^{me} \\ \mathbb{P}^{e} \\ \mathbb{P}^{me+1} \\ \mathbb{P}^{e} \\ \mathbb{P}^{e+1} \\ \mathbb{$$





Gradient flow and NTK - summary

$$\begin{aligned} \dot{\theta} &= -\eta \nabla_{\theta} f_{\mathcal{D}} \nabla_{f} \mathcal{L}_{\mathcal{D}} \\ \dot{f}_{\mathcal{D}} &= -\eta G \nabla_{f} \mathcal{L} \\ \varsigma(x, x') &= \nabla_{\theta} f(x)^{T} \nabla_{\theta} f(x') \end{aligned}$$

• f_X , $\nabla_{\theta} f_X$, G depend only on the inputs X, θ

- ▶ $\nabla_f \mathcal{L}$ depends only on the correct outputs Y, and predicted outputs, i.e. on Y and θ
- This holds for any predictor! So what is special about neural networks?

Gradient flow and NTK – summary

$$\begin{split} \dot{\theta} &= -\eta \nabla_{\theta} f_{\mathcal{D}} \nabla_{f} \mathcal{L}_{\mathcal{D}} \quad \in \mathbb{R}^{p} \\ \dot{f}_{\mathcal{D}} &= -\eta G \nabla_{f} \mathcal{L} \quad \in \mathbb{R}^{p} \\ \kappa(x, x') &= \nabla_{\theta} f(x)^{T} \nabla_{\theta} f(x') \end{split}$$

• f_X , $\nabla_{\theta} f_X$, G depend only on the inputs X, θ

- ▶ $\nabla_f \mathcal{L}$ depends only on the correct outputs Y, and predicted outputs, i.e. on Y and θ
- This holds for any predictor! So what is special about neural networks?
- First, we will analyze κ for very wide neural networks with random parameters (e.g. at initialization)
 Then we will analyze what happens during training under assumption (A3)
 (i) m_{1,1} → ∞ ⇒ K^{1:L} betterminisfic

Wide NN's Gaussian Process (GP)

- This is about f₀, a NN initialized with Gaussian independent parameters. For simplicity, we denote it as f.
- Assume $\theta^{1:L-1}$ fixed, only W^L , b^L random as in (??) Recall $f(x) = W^L x^{L-1}(x) + b^L$ for any x with $x^{L-1} \in \mathbb{R}^{m_L}$
- $P = \operatorname{Recall} r(x) = W + x + (x) + b = \operatorname{Recall} x + \operatorname{Recall} x + c = \mathbb{R}^{-1}$
- ▶ $f(x) = \text{sum of } m_{L-1} \text{ i.i.d. random variables, hence } f(x) \sim Normal \text{ by CLT, for } m_{L-1} \text{ large}$ ▶ Randomness is over weights W^L, b^L !!!
- We have E[f(x)] = 0 and

$$Cov(f(x), f(x')) = E[(W^{L}x^{L-1} + b^{L})(W^{L}(x')^{L-1} + b^{L})] = \frac{\sigma_{w}^{2}}{m_{L-1}}(x^{L-1})^{T}(x')^{L-1} + \sigma_{b}^{2} \equiv \kappa^{L}(x^{L-1})^{T}(x')^{L-1} + \sigma_{b}^{2} \equiv \kappa^{L}(x^{L-1})^{T}(x')^{T}(x')^{T}(x')^{L-1} + \sigma_{b}^{2} \equiv \kappa^{L}(x^{L-1})^{T}(x')^{$$

where x^{L-1} , $(x')^{L-1} \in \mathbb{R}^{m_{L-1}}$ are the outputs of the (L-1)-th layer for inputs x, x'

- κ^{L} is a positive definite kernel Exercise Prove this.
- f(x) is a random function of x
- The distribution of f(x) defined as above, is called a Gaussian Pocess
- More generally, it can be shown [Jacot, Gabriel, Hongler, NeurIPS 2018] that, when all θ parameters are sampled as in (??), $f_0(x) \sim GP(0, \kappa^L)$
- Q1 What is the kernel κ^{L} of this GP
- Q2 This is all nice, but θ changes during training. What can we say about θ_t , f_t after training?

Q1: Idea.

(i)

From (8), for layer l = 1 : L we have

$$\kappa^{\prime}(x,x') = E[z_{j}^{\prime}(x)z_{j}^{\prime}(x')] = \frac{\sigma_{w}^{2}}{m_{l-\frac{1}{2}}}(x^{\prime-1})^{T}(x')^{\prime-1} + \sigma_{b}^{2}$$
(9)

with $x^{l-1} = \phi(z^{l-1})$. Note also that z_j^l are i.i.d. so it does not matter which j we choose.

- ▶ In particular, $\kappa^1(x, x') = \frac{\sigma_w^2}{m_1} x^T x' + \sigma_b^2$ is deterministic
- ... and κ^l is random for l > 1.
- However, when $m_l \to \infty$, $\frac{1}{m_{l-=}} (x^{l-1})^T (x')^{l-1} \to E[*]$
- More specifically, this expectation can be written as

$$E[*] = \int \int \phi(z)\phi(z') Normal(\begin{bmatrix} z \\ z' \end{bmatrix}; 0, \kappa_{x,x'}^{l-1}) dz dz'.$$
(10)

In the above z, z' represent the $z^{l-1}(x), z^{l-1}(x')$ variables, sampled from the level lNormal distribution, which has covariance given by κ^{l-1} , namely

$$\kappa_{\mathbf{x},\mathbf{x}'}^{l-1} = \begin{bmatrix} \kappa^{l-1}(\mathbf{x},\mathbf{x}) & \kappa^{l-1}(\mathbf{x},\mathbf{x}') \\ \kappa^{l-1}(\mathbf{x}',\mathbf{x}) & \kappa^{l-1}(\mathbf{x}',\mathbf{x}') \end{bmatrix}.$$
 (11)

• Hence, the limit of $\kappa^{I}(\mathbf{x}, \mathbf{x}')$ when $m_{1:I} \to \infty$, is a deterministic kernel for all *I*. [Jacot, Gabriel, Hongler, NeurIPS 2018] derived this recursion (next page).

Q1: A recursive expression for the Neural Tangent Kernel

[Jacot, Gabriel, Hongler, NeurIPS 2018]

- *L* fixed, $m \to \infty$
- Simplified expression for $m_{0:L} = m$, $\sigma_w = \sigma_b = 1$
- Then the NTK $\kappa \equiv \kappa^L$ is defined recursively by layer

$$\kappa^{1}(x,x') = \Sigma^{1}(x,x'), \quad \Sigma^{1}(x,x') = \frac{1}{m}x^{T}x' + 1$$
 (12)

$$\kappa^{l+1}(x,x') = \kappa^{l}(x,x')\dot{\Sigma}^{l+1}(x,x') + \Sigma^{l+1}(x,x'), \tag{13}$$

with

$$\Sigma^{l+1}(x, x') = \mathsf{L}^{\phi}_{\Sigma^{l}(x, x')},\tag{14}$$

$$\dot{\Sigma}^{l+1}(x, x') = \mathsf{L}^{\phi'}_{\Sigma^{l}(x, x')},\tag{15}$$

and

 $\mathsf{L}_{\Sigma}^{\phi} = E[\phi(X)\phi(X')] \operatorname{with}(X,X') \sim \mathsf{N}(0, \begin{bmatrix} \Sigma(X,X) & \Sigma(X,X') \\ \Sigma(X,X') & \Sigma(X',X') \end{bmatrix} (16)$

▶ In other words, at level l + 1, $X \equiv x^l, X' \equiv (x')^l$ are sampled from a GP with kernel Σ^l , and $\Sigma^{l+1}(x, x')$, $\dot{\Sigma}^{l+1}(x, x')$ represent their (scalar) covariance after passing through the non-linearities ϕ , ϕ' (where ϕ' is the derivative of ϕ)

Summary so far

Now, we understand the random intialization of wide networks, with *L* layers.

$$f_0 \sim GP(0, \kappa^L)$$

(17)

where κ^{L} is a kernel that depends only on ϕ (and $\sigma^{2}_{b,w}$)

What next?

- Analysis of training by linearization iii
- ▶ Then, the NTK limit for $L \rightarrow \infty$ and its relevance for classification and regression

The Linearized Network f^{lin}

Notation: $\theta_{0,t}$, $f_{0,t}$ = parameters, predictor at times 0, t

too in a A

Here we use (A3), the assumption that the parameters θ change little during training. Extensive evidence supports this assumption.

First order Taylor expansion of f_t around f_0

$$\lim_{x \to 0} f_0(x) + \nabla_\theta f_0(x)^T (\theta_t - \theta_0) \xrightarrow{\simeq} f \qquad (18)$$

$$\nabla_{\theta} f_t^{\text{lin}} = \nabla_{\theta} f_0 \tag{19}$$

$$\kappa(x, x') = \nabla_{\theta} f_0(x)^T \nabla_{\theta} f_0(x') \quad \text{constant during training} \qquad (20)$$

$$G_0 \equiv \kappa_{X,X} = \text{NTK of random vel} \qquad (21)$$

$$\dot{\theta}_t = -\eta \nabla_{\theta} f_0(\mathsf{X})^T \nabla_f \mathcal{L}(\mathsf{Y}, f_t^{\mathrm{lin}}(\mathsf{x}))$$
(22)

$$^{\text{in}}(x) = -\eta \underbrace{\kappa(x, X) G_0}_{\text{depends on } \theta_0} \nabla_f \mathcal{L}(Y, f_t^{\text{lin}}(x))$$
(23)

NTK during training - empirical evidence

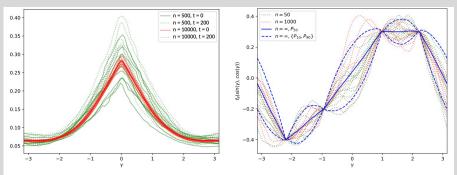


Figure 1: Convergence of the NTK to a fixed limit Figure 2: Networks function f_{θ} near convergence for two widths n and two times t. for two widths n and two times t.

Linearized Network dynamics for \mathcal{L}_{LS}

For example, for $\mathcal{L}_{LS}(y, f) = \frac{1}{2}(f - y)^2$, $\nabla_f \mathcal{L}_{LS}(f, y) = f - y$. In this case, equations (??) are a linear system and have an analytic solution.

$$_{t} - \theta_{0} = -\nabla_{\theta} f_{0}(\mathsf{X})^{T} G_{0}^{-1} \left(I - e^{-\eta G_{0} t} \right) \left(f_{0}(\mathsf{X}) - \mathsf{Y} \right)$$
(24)

$$\lim_{t \to \infty} (\mathsf{X}) = \left(I - e^{-\eta G_0 t} \right) \mathsf{Y} + e^{-\eta G_0 t} f_0(\mathsf{X})$$
(25)

$$f_t^{\text{lin}}(x) = \underbrace{\kappa(x, X)^T G_0^{-1} \left(I - e^{-\eta G_0 t} \right) Y}_{\mu(x)} + \underbrace{f_0(x) - \kappa(x, X)^T G_0^{-1} \left(I - e^{-\eta G_0 t} \right) f_0(\underline{k26})}_{\gamma(x)}$$

Notes:

θ

- if $G_0 \succ 0$ then $e^{-\eta G_0 t} \rightarrow 0$ for $t \rightarrow \infty$
- ▶ in discrete time t = 0, 1, 3, ... replace e^{at} with $(1 a)^t$. Sketch of proof: $\ln(1 - a)^t = t \ln(1 - a) \approx t(-a)$ for a small; therefore $e^{-at} \approx (1 - a)^t$.
- $f_t^{\text{lin}}(x) = f_0(x) + \kappa(x, X)^T G_0^{-1} \left(I e^{-\eta G_0 t} \right) (Y f_0(X))$

Exercise Prove (??) from (??)

Wide and deep neural networks for classification – Basic quantities and assumptions

[Radhakrishnan, Belkin, Ulher, 2022]

- ▶ This paper studies the limits of wide neural networks $m_l \to \infty$ for all l = 1 : L when the depth $L \to \infty$
- ▶ It is already known that for regression $L \rightarrow \infty$ is NOT OPTIMAL
- Since the NTK depends only of the activation function φ, the limit shall only depend on φ as well.
- In particular, the limit depends on ϕ only through the following

$$A = E[\phi(Z)] \qquad \text{when } z \sim N(0,1)$$

$$A' = E[\phi'(Z)] \qquad \text{when } z \sim N(0,1)$$

$$B = E[(\phi'(Z))^2] \qquad \text{when } z \sim N(0,1)$$

- Classifier $f(x) = \lim_{L \to \infty} \operatorname{sgn} Y G^{-1} \kappa^{L}(X, x)$ with $G = [\kappa^{L}(x^{i}, x^{j})]_{i,j=1:n}$.
- Additional assumptions
 - Data $X \subseteq S^d_+$, vectors of norm 1 with all entries ≥ 0 .
 - Simplifying assumptions on NTK parameters (e.g. $\sigma_w = \sigma_b = 1$)

$${}^{"}{\mathcal{K}}^{L} \longrightarrow {}^{"}{\mathcal{O}} \Leftarrow L \rightarrow \infty$$

informal statement

Case $A \neq 0$: Networks implement majority vote

Theorem (Proposition 1 in [Radhakrishnan, Belkin, Ulher, 2022]) If there is a function $0 < c(L) < \infty$ so that

$$\lim_{L \to \infty} \frac{\kappa^{L}(x, x')}{c(L)} = c_1 > 0 \text{ for any } x \neq x', \text{ and } \lim_{L \to \infty} \frac{\kappa^{L}(x, x)}{c(L)} \neq c_1,$$
(27)

then

$$\lim_{L \to \infty} f(x) = \operatorname{sgn} \sum_{i=1}^{n} y^{i} \qquad MAJORITY \ CLASSIFIER$$
(28)

• What ϕ 's satisfy theorem? ReLU, all ϕ with $B \neq 1$.



Case A = A' = 0: Networks implement 1-nearest neighbor

Theorem (Theorem 3 in [Radhakrishnan, Belkin, Ulher, 2022]) Given x, assume w.l.o.g. that $x^T x^1 = \max_{i=1:n} x^T x^i$.

$$\lim_{t \to \infty} \frac{\kappa^L(x, x^i)}{\kappa^L(x, x^1)} = 0.$$
⁽²⁹⁾

and

$$\lim_{L \to \infty} f(x) = \operatorname{sgn} y^1 \qquad 1-nn \tag{30}$$



Case A = 0, $A' \neq 0$: Networks implement singular kernel classifier

Theorem (Theorem 1 in [Radhakrishnan, Belkin, Ulher, 2022])

$$\lim_{t \to \infty} \frac{\kappa^{L}(x, x')}{(A')^{2L}(L+1)} = \frac{R(||x - x'||)}{||x - x'||^{\alpha}},$$
(31)

with $\alpha = -4 \frac{\log A'}{\log B'}$ and $R() \ge 0$, bounded, and $R(u) > \delta$ around 0.

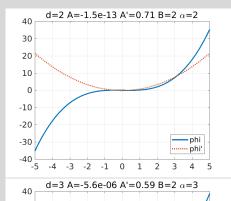
- ▶ if $\alpha > 0$, $\frac{R(||x-x'||)}{||x-x'||^{\alpha}}$ is singular kernel
- Computationally not a problem: if data x^{1:n} distinct, G₀ is well defined
 If x = xⁱ, set f(x) = yⁱ.

Optimality of singular kernel classifier

Theorem (Theorem 2 in [Radhakrishnan, Belkin, Ulher, 2022]) If A = 0, $A' \neq 0$ and $\alpha = +d$ then $\lim_{L\to\infty} f(x)$ is Bayes-optimal.

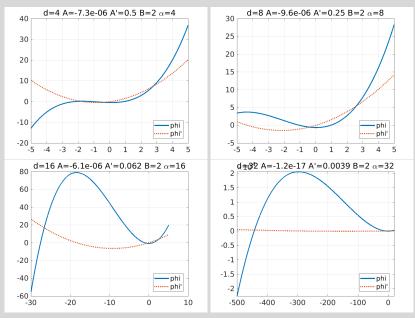
• What activations ϕ satisfy this theorem?

$$\phi^{\text{opt}}(z) = \frac{1}{2^{d/4}} \frac{z^3 - 3z}{\sqrt{6}} + \sqrt{1 - 2^{1 - d/2}} \frac{z^2 - 1}{\sqrt{2}} + \frac{1}{2^{d/4}} z \quad \text{for } d \ge 2$$
(32)

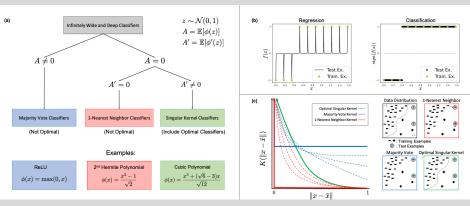


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Optimal singular kernels for d = 4, 8, 16, 32



Summary



b when A ≠ 0, lim_{L→∞} κ^L(x, x') = 0 for x ≠ x', and f(x) = 0 is vanishingly small (useless for regression), but sgnf(x) can be optimal for classification
 c Singular kernel α > d, α < d, majority vote kernel, and 1-nn kernel

Limits of some activation functions

