On Exact Computation with an Infinitely Wide Neural Net

Sanjeev Arora[*]   Simon S. Du[†]   Wei Hu[‡]   Zhiyuan Li[§]

Ruslan Salakhutdinov[¶]   Ruosong Wang[‖]

Abstract

How well does a classic deep net architecture like AlexNet or VGG19 classify on a standard dataset such as CIFAR-10 when its "width"— namely, number of channels in convolutional layers, and number of nodes in fully-connected internal layers — is allowed to increase to infinity? Such questions have come to the forefront in the quest to theoretically understand deep learning and its mysteries about optimization and generalization. They also connect deep learning to notions such as *Gaussian processes* and *kernels*. A recent paper [Jacot et al., 2018] introduced the *Neural Tangent Kernel (NTK)* which captures the behavior of fully-connected deep nets in the infinite width limit trained by gradient descent; this object was implicit in some other recent papers. A subsequent paper [Lee et al., 2019] gave heuristic Monte Carlo methods to estimate the NTK and its extension, *Convolutional Neural Tangent Kernel (CNTK)*, and used this to try to understand the limiting behavior on datasets like CIFAR-10. An attraction of such ideas is that a pure kernel-based method is used to capture the power of a fully-trained deep net of infinite width.

The current paper gives the first efficient exact algorithm (based upon dynamic programming) for computing CNTK as well as an efficient GPU implementation of this algorithm. This results in a significant new benchmark for performance of a pure kernel-based method on CIFAR-10, being 10% higher than the methods reported in [Novak et al., 2019], and only 5% lower than the performance of the corresponding finite deep net architecture (once batch normalization etc. are turned off).

We give the first *non-asymptotic* proof showing that a fully-trained sufficiently wide net is indeed equivalent to the kernel regression predictor using NTK. Our experiments also demonstrate that earlier Monte Carlo approximation can degrade the performance significantly, thus highlighting the power of our exact kernel computation, which we have applied even to the full CIFAR-10 dataset and 20-layer nets.

1 Introduction

How well does a classic deep net architecture like AlexNet or VGG19 perform on a standard dataset such as CIFAR-10 when its "width"— namely, number of channels in convolutional layers, and number of nodes in fully-connected internal layers — is allowed to increase to infinity? Questions

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[*]Princeton University and Institute for Advanced Study. Email: arora@cs.princeton.edu

[†]Carnegie Mellon University. Email: ssdu@cs.cmu.edu

[‡]Princeton University. Email: huwei@cs.princeton.edu

[§]Princeton University. Email: zhiyuanli@cs.princeton.edu

[¶]Carnegie Mellon University. Email:rsalakhu@cs.cmu.edu

[‖]Carnegie Mellon University. Email: ruosongw@andrew.cmu.edu

about these "infinite limits" of deep nets have naturally emerged in the ongoing effort to understand the power of deep learning. In mathematics it is often easier to study objects in the infinite limit. Furthermore, the infinite limit could conceivably make sense in deep learning, since *over-parametrization* seems to help optimization a lot and doesn't hurt generalization much [Zhang et al., 2017]: deep neural nets with millions of parameters work well even for datasets with 50k training data points. So why not imagine nets whose width goes to infinity?

Allowing width to go to infinity also connects deep learning in an interesting way with other areas of machine learning. 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]. This model as well as analogous ones with multiple layers [Lee et al., 2018, Matthews et al., 2018] and convolutional filters [Novak et al., 2019, Garriga-Alonso et al., 2019] make up the Gaussian Process view of deep learning. These correspond to infinitely wide deep nets whose all parameters are chosen randomly (with careful scaling), and only the top (classification) layer is trained.

From now on we will use *weakly-trained nets* to refer to nets whose layers receive random initialization and only the top layer is trained by gradient descent. We use *fully-trained* to refer to nets whose all parameters are trained. It has long been known that weakly-trained convolutional nets have reasonable performance on MNIST and CIFAR-10. Weakly-trained nets that are fully-connected instead of convolutional, can also be thought of as "multi-layer random kitchen sinks," which also have a long history.

Weakly-trained nets — whether of finite or infinite width — also define interesting kernels. Specifically, if $f(\boldsymbol{\theta}, \boldsymbol{x}) \in \mathbb{R}$ denotes the output of the network on input $\boldsymbol{x}$ where $\boldsymbol{\theta}$ denotes the parameters in the network, and $\mathcal{W}$ is an initialization distribution over $\boldsymbol{\theta}$ (usually Gaussian), then training just the top layer with an ℓ_2 loss is equivalent to a kernel regression for the following kernel:

$$\ker\left(\boldsymbol{x}, \boldsymbol{x}'\right) = \mathbb{E}_{\boldsymbol{\theta} \sim \mathcal{W}}[f\left(\boldsymbol{\theta}, \boldsymbol{x}\right) \cdot f\left(\boldsymbol{\theta}, \boldsymbol{x}'\right)], \tag{1}$$

where $\boldsymbol{x}, \boldsymbol{x}'$ are two inputs. This kernel method makes sense even if the number of parameters goes to infinity.

The objects of interest in this paper are not weakly-trained nets, but fully-trained nets. In the finite case, analysis of optimization and generalization of fully-trained nets is of course an open problem. One may also ask:

Can we understand the power of fully-trained nets whose width goes to infinity?

A priori this question doesn't seem any easier than the finite case, and empirical evaluation seems computationally infeasible due to the infinite limit. They also do not correspond to a kernel method in any obvious way.

Recent papers suggest that nets whose width greatly exceeds the number of training data points can rapidly reduce training error to 0 via gradient descent, and under some conditions, the trained net also exhibits good generalization [Du et al., 2019, 2018b, Li and Liang, 2018, Allen-Zhu et al., 2018a,b, Zou et al., 2018, Arora et al., 2019]. Extra-wideness plays a crucial role in the proof: it is shown that as width increases, training causes increasingly smaller changes (in a proportionate sense) in the parameters. This raises the possibility that as one increases the width to infinity, a certain limiting behavior can emerge even in the fully-trained net. A recent paper by Jacot et al. [2018] isolated a notion implicit in the above papers [Du et al., 2019, 2018b], which they called the *Neural Tangent Kernel (NTK)*. They suggested — via a proof that is slightly heuristic — that this fixed kernel characterizes the behavior of fully-connected infinite width neural networks whose

layers have been trained by gradient descent. The NTK is very different from the Gaussian Process kernels discussed earlier, and is defined using the *gradient* of the output of the randomly initialized net with respect to its parameters, i.e.,

$$\ker\left(\boldsymbol{x}, \boldsymbol{x}'\right) = \mathop{\mathbb{E}}_{\boldsymbol{\theta} \sim \mathcal{W}} \left\langle \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{\theta}}, \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \boldsymbol{\theta}} \right\rangle. \tag{2}$$

Here, the gradient $\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{\theta}}$ appears from considering gradient descent, as will be explained in Section 3. One may also generalize the NTK to convolutional neural nets, and we call the corresponding kernel *Convolutional Neural Tangent Kernel (CNTK)*.

Though NTK and CNTK are defined by an infinite limit, a recent paper [Lee et al., 2019] attempted to understand their properties via a heuristic finite approximation of the infinite limit kernel by Monte Carlo methods. However, as will be shown in Section 5.2, such Monte Carlo methods can degrade the performance a lot. It was still open what is the full power of *exact* NTK and CNTK on modern datasets. This is a challenging question especially for CNTK, since when convolutional operation is involved, it is believed that exact computation of kernels (for either convolutional Gaussian Process kernel or CNTK) is infeasible for large datasets like CIFAR-10 [Novak et al., 2019].

Our Contributions. We give an exact and efficient dynamic programming algorithm to compute the NTK and CNTK for ReLU activation (namely, to compute $\ker\left(\boldsymbol{x}, \boldsymbol{x}'\right)$ given $\boldsymbol{x}$ and $\boldsymbol{x}'$). Using this algorithm — as well as implementation tricks for GPUs — we can settle the question of the performance of fully-trained infinitely wide nets with a variety of architectures. For instance, we find that their performance on CIFAR-10 is within 5% of the performance of the same architectures in the finite case (note that the proper comparison in the finite case involves turning off batch norm, data augmentation, dropout, etc., in the optimization). In particular, the CNTK corresponding to a 10-layer convolutional net with global averge pooling achieves 77% classification accuracy. This is 10% higher than the best reported performance of a Gaussian process with fixed kernel on CIFAR-10 [Novak et al., 2019]. [1]

We give a more rigorous, non-asymptotic proof that the NTK captures the behavior of a fully-trained wide neural net under weaker condition than previous proofs. We also experimentally show that the Monte Carlo methods for approximating CNTK in the earlier work do not compute good approximations, which is clear from their much worse performance on CIFAR.

1.1 Notation

We use bold-faced letters for vectors, matrices and tensors. For a vector $\boldsymbol{a}$, let $[\boldsymbol{a}]_i$ be its i-th entry; for a matrix $\boldsymbol{A}$, let $[\boldsymbol{A}]_{i,j}$ be its (i,j)-th entry; for a 4th-order tensor $\boldsymbol{T}$, let $[\boldsymbol{A}]_{ij,i'j'}$ be its (i,j,i',j')-th entry. Let $\boldsymbol{I}$ be the identity matrix, and $[n] = \{1, 2, \dots, n\}$. Let $\boldsymbol{e}_i$ be an indicator vector with i-th entry being 1 and other entries being 0, and let $\boldsymbol{1}$ denote the all-one vector. We use $\odot$ to denote the pointwise product and $\otimes$ to denote the tensor product. We use $\text{diag}(\cdot)$ to transform a vector to a diagonal matrix. We use $\sigma(\cdot)$ to denote the activation function, such as the rectified linear unit (ReLU) function: $\sigma(z) = \max\{z, 0\}$, and $\dot{\sigma}(\cdot)$ to denote the derivative of $\sigma(\cdot)$. Denote by $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ the Gaussian distribution with mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$.

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[1] We only consider fixed kernels defined without using the training data. We do not compare to methods that tune the kernels using training data [Van der Wilk et al., 2017] or use a neural network to extract features and then applying a kernel method on top of them [Mairal et al., 2014].

1.2 Paper Organization

The rest of the paper is organized as follows. Section 2 gives an overview of related work. In Section 3, we review how NTK arises from training an infinitely wide fully-connected neural network, and also rigorously establish the equivalence between a fully-trained wide neural net and kernel regression under the NTK. In Section 4, we derive the formulas for CNTK, and describe our efficient computation of CNTK; In Section 5, we present our experimental results and discuss our findings. Lastly, we conclude in Section 6.

2 Related Work

From a Gaussian Process (GP) viewpoint, the correspondence between infinite neural networks and kernel machines was first noted by Neal [1996]. Follow-up work extended this correspondence to more general shallow neural networks [Williams, 1997, Roux and Bengio, 2007, Hazan and Jaakkola, 2015]. More recently, this was extended to deep and convolutional neural networks [Lee et al., 2018, Matthews et al., 2018, Novak et al., 2019, Garriga-Alonso et al., 2019]. However, these kernels, as we discussed in Section 1, represent weakly-trained nets, instead of fully-trained nets.

Beyond GPs, the connection between neural networks and kernels is also studied in the compositional kernel literature. Cho and Saul [2009] derived a closed-form kernel formula for rectified polynomial activations, which include ReLU as a special case. Daniely et al. [2016] proposed a general framework to transform a neural network to a compositional kernel and later Daniely [2017] showed for sufficiently wide neural networks, stochastic gradient descent can learn functions that lie in the corresponding reproducing kernel Hilbert space. However, the kernels studied in these works still correspond to weakly-trained neural networks.

Wilson et al. [2016], Al-Shedivat et al. [2016] used a neural network as a feature extractor, applied a GP on top of these features and then trained the resulting model end-to-end. Another line of work built probabilistic graphical models (PGMs) which uses kernel as a component [Damianou and Lawrence, 2013, Lawrence and Moore, 2007, Van der Wilk et al., 2017, Kumar et al., 2018, Blomqvist et al., 2018]. These are not pure kernel methods so we do not compare with them in this paper. Nevertheless, CNTK may be combined with these techniques to generate more powerful predictors.

This paper is inspired by a line of recent work on over-parameterized neural networks [Du et al., 2019, 2018b, Du and Hu, 2019, Li and Liang, 2018, Allen-Zhu et al., 2018b,a, Zou et al., 2018]. These papers established that for (convolutional) neural networks with large but finite width, (stochastic) gradient descent can achieve zero training error. A key component in these papers is showing that the weight matrix at each layer is close to its initialization. This observation implies that the kernel defined in Equation (2) is still close to its initialization. Arora et al. [2019] explicitly used this observation to derive generalization bounds for two-layer over-parameterized neural networks.

Jacot et al. [2018] derived the exact same kernel from kernel gradient descent. They showed that if the number of neurons per layer goes to infinity in a sequential order, then the kernel remains unchanged for a finite training time. They termed the derived kernel *Neural Tangent Kernel (NTK)*. We follow the same naming convention and name its convolutional extension *Convolutional Neural Tangent Kernel (CNTK)*. Later, Yang [2019] derived a formula of CNTK. Comparing with [Yang, 2019], our CNTK formula has a more explicit convolutional structure and results in an efficient GPU-friendly computation method. Recently, Lee et al. [2019] tried to empirically verify the theory

in [Jacot et al., 2018] using a heuristic Monte Carlo method. They showed that in the first few iterations, the kernel is approximately unchanged. However, as will be shown in Section 5.2, such Monte Carlo methods can decrease the classification accuracy by 5% even on a "CIFAR-2" (airplane V.S. car) dataset. Therefore, exact kernel evaluation is important to study the power of NTK and CNTK.

3 Neural Tangent Kernel

In this section we describe fully-connected deep neural net architecture and its infinite width limit, and how training it with respect to the ℓ_2 loss gives rise to a kernel regression problem involving the neural tangent kernel (NTK).

We denote by $f(\boldsymbol{\theta}, \boldsymbol{x}) \in \mathbb{R}$ the output of a neural network where $\boldsymbol{\theta} \in \mathbb{R}^N$ is all the parameters in the network and $\boldsymbol{x} \in \mathbb{R}^d$ is the input.[2] Given a training dataset $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \subset \mathbb{R}^d \times \mathbb{R}$, consider training the neural network by minimizing the squared loss over training data:

$$\ell(\boldsymbol{\theta}) = \frac{1}{2} \sum_{i=1}^n \left(f(\boldsymbol{\theta}, \boldsymbol{x}_i) - y_i \right)^2.$$

The proof of the following lemma uses simple differentiation and appears in Appendix A.

Lemma 3.1. *Consider minimizing the squared loss $\ell(\boldsymbol{\theta})$ by gradient descent with infinitesimally small learning rate: $\frac{\mathrm{d}\boldsymbol{\theta}(t)}{\mathrm{d}t} = -\nabla\ell(\boldsymbol{\theta}(t))$. Let $\boldsymbol{u}(t) = (f(\boldsymbol{\theta}(t), \boldsymbol{x}_i))_{i\in[n]} \in \mathbb{R}^n$ be the network outputs on all $\boldsymbol{x}_i$'s at time t, and $\boldsymbol{y} = (y_i)_{i\in[n]}$ be the desired outputs. Then $\boldsymbol{u}(t)$ follows the following evolution, where $\boldsymbol{H}(t)$ is an $n \times n$ positive semidefinite matrix whose (i,j)-th entry is $\left\langle \frac{\partial f(\boldsymbol{\theta}(t), \boldsymbol{x}_i)}{\partial \boldsymbol{\theta}}, \frac{\partial f(\boldsymbol{\theta}(t), \boldsymbol{x}_j)}{\partial \boldsymbol{\theta}} \right\rangle$:*

$$\frac{\mathrm{d}\boldsymbol{u}(t)}{\mathrm{d}t} = -\boldsymbol{H}(t) \cdot (\boldsymbol{u}(t) - \boldsymbol{y}). \tag{3}$$

The statement of Lemma 3.1 involves a matrix $\boldsymbol{H}(t)$. Below we define a deep net architecture whose width is allowed to go to infinity, while fixing the training data as above. In the limit, it can be shown that the matrix $\boldsymbol{H}(t)$ remains *constant* during training i.e., equal to $\boldsymbol{H}(0)$. Moreover, under a random initialization of parameters, the random matrix $\boldsymbol{H}(0)$ converges in probability to a certain deterministic kernel matrix $\boldsymbol{H}^*$ as the width goes to infinity, which is the *Neural Tangent Kernel* $\ker(\cdot, \cdot)$ (Equation (2)) evaluated on the training data. If $\boldsymbol{H}(t) = \boldsymbol{H}^*$ for all t, then Equation (3) becomes

$$\frac{\mathrm{d}\boldsymbol{u}(t)}{\mathrm{d}t} = -\boldsymbol{H}^* \cdot (\boldsymbol{u}(t) - \boldsymbol{y}). \tag{4}$$

Note that the above dynamics is identical to the dynamics of *kernel regression* under gradient flow, for which at time $t \to \infty$ the final prediction function is (assuming $\boldsymbol{u}(0) = \boldsymbol{0}$)

$$f^*(\boldsymbol{x}) = (\ker(\boldsymbol{x}, \boldsymbol{x}_1), \dots, \ker(\boldsymbol{x}, \boldsymbol{x}_n)) \cdot (\boldsymbol{H}^*)^{-1}\boldsymbol{y}. \tag{5}$$

In Theorem 3.2, we rigorously prove that a fully-trained sufficiently wide ReLU neural network is equivalent to the kernel regression predictor (5) on any given data point.

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[2]For simplicity, we only consider a single output here. The generalization to multiple outputs is straightforward.

3.1 Fully-Connected Deep Neural Net and Its Infinite Width Limit

Now we define fully-connected deep neural net and review its Gaussian Process viewpoint in the infinite width limit. Fully-connected net is defined in the standard way: the h-th layer is computed by applying a linear transformation on the output of the $(h-1)$-th layer, followed by a coordinate-wise nonlinearity σ. Recall that standard initialzion would pick each entry of the layer matrix from $\mathcal{N}(0, \delta^2)$ where δ is such that the expected norm of each row in the matrix is 1. Thus δ depends on the number of nodes in the row, and the initialization stays bounded as we let the number of nodes in each row go to infinity.

The limit behavior of gradient descent depends however on the details of initialization. In this paper we initialize parameters using $\mathcal{N}(0, 1)$ and multiply δ on the outside (instead of using $\mathcal{N}(0, \delta^2)$ to initialize). These two parameterizations can be made equivalent if one is allowed to set different learning rates for different layers, as discussed in [Lee et al., 2019]. In fact the gradient from each layer defines a different kernel, and setting different learning rates for different layers amounts to summing over those individual kernels with different weights. Our choice allows setting equal learning rates for all the layers while giving rise to the NTK in the infinite width limit, which is the unweighted sum of those individual kernels. In contrast, using Kaiming initialization [He et al., 2015] at infinite width is equivalent to setting the learning rate of the first layer to 0 and the rest to be equal, thus resulting in a similar kernel to the NTK — the unweighted sum of kernels from the second layer to the last layer. The initialization method in [Daniely, 2017] gives the kernel corresponding to the last layer only, which corresponds to Gaussian process.

Now we define a fully-connected neural net formally. Let $\boldsymbol{x} \in \mathbb{R}^d$ be the input, and denote $\boldsymbol{g}^{(0)}(\boldsymbol{x}) = \boldsymbol{x}$ and $d_0 = d$ for notational convenience. We define an L-hidden-layer fully-connected neural network recursively:

$$\boldsymbol{f}^{(h)}(\boldsymbol{x}) = \boldsymbol{W}^{(h)}\boldsymbol{g}^{(h-1)}(\boldsymbol{x}) \in \mathbb{R}^{d_h}, \quad \boldsymbol{g}^{(h)}(\boldsymbol{x}) = \sqrt{\frac{c_\sigma}{d_h}}\sigma\left(\boldsymbol{f}^{(h)}(\boldsymbol{x})\right) \in \mathbb{R}^{d_h}, \qquad h = 1, 2, \ldots, L, \quad (6)$$

where $\boldsymbol{W}^{(h)} \in \mathbb{R}^{d_h \times d_{h-1}}$ is the weight matrix in the h-th layer ($h \in [L]$), $\sigma : \mathbb{R} \to \mathbb{R}$ is a coordinate-wise activation function, and $c_\sigma = \left(\mathbb{E}_{z \sim \mathcal{N}(0,1)}\left[\sigma(z)^2\right]\right)^{-1}$. The last layer of the neural network is

$$\begin{aligned} f(\boldsymbol{\theta}, \boldsymbol{x}) = f^{(L+1)}(\boldsymbol{x}) &= \boldsymbol{W}^{(L+1)} \cdot \boldsymbol{g}^{(L)}(\boldsymbol{x}) \\ &= \boldsymbol{W}^{(L+1)} \cdot \sqrt{\frac{c_\sigma}{d_L}}\sigma\left(\boldsymbol{W}^{(L)} \cdot \sqrt{\frac{c_\sigma}{d_{L-1}}}\sigma\left(\boldsymbol{W}^{(L-1)} \cdots \sqrt{\frac{c_\sigma}{d_1}}\sigma\left(\boldsymbol{W}^{(1)}\boldsymbol{x}\right)\right)\right), \end{aligned}$$

where $\boldsymbol{W}^{(L+1)} \in \mathbb{R}^{1 \times d_L}$ is the weights in the final layer, and $\boldsymbol{\theta} = \left(\boldsymbol{W}^{(1)}, \ldots, \boldsymbol{W}^{(L+1)}\right)$ represents all the parameters in the network.

We initialize all the weights to be i.i.d. $\mathcal{N}(0, 1)$ random variables, and consider the limit of large hidden widths: $d_1, d_2, \ldots, d_L \to \infty$. The scaling factor $\sqrt{c_\sigma/d_h}$ in Equation (6) ensures that the norm of $\boldsymbol{g}^{(h)}(\boldsymbol{x})$ for each $h \in [L]$ is approximately preserved at initialization (see [Du et al., 2018b]). In particular, for ReLU activation, we have $\mathbb{E}\left[\left\|\boldsymbol{g}^{(h)}(\boldsymbol{x})\right\|^2\right] = \|\boldsymbol{x}\|^2$ ($\forall h \in [L]$).

Recall from [Lee et al., 2018] that in the infinite width limit, the pre-activations $\boldsymbol{f}^{(h)}(\boldsymbol{x})$ at every hidden layer $h \in [L]$ has all its coordinates tending to i.i.d. centered Gaussian processes of

covariance $\Sigma^{(h-1)} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ defined recursively as:

$$
\begin{aligned}
\Sigma^{(0)}(\boldsymbol{x}, \boldsymbol{x}') &= \boldsymbol{x}^\top \boldsymbol{x}', \\
\boldsymbol{\Lambda}^{(h)}(\boldsymbol{x}, \boldsymbol{x}') &= \begin{pmatrix} \Sigma^{(h-1)}(\boldsymbol{x}, \boldsymbol{x}) & \Sigma^{(h-1)}(\boldsymbol{x}, \boldsymbol{x}') \\ \Sigma^{(h-1)}(\boldsymbol{x}', \boldsymbol{x}) & \Sigma^{(h-1)}(\boldsymbol{x}', \boldsymbol{x}') \end{pmatrix} \in \mathbb{R}^{2 \times 2}, \\
\Sigma^{(h)}(\boldsymbol{x}, \boldsymbol{x}') &= c_\sigma \mathop{\mathbb{E}}_{(u,v) \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Lambda}^{(h)})} \left[\sigma(u) \sigma(v) \right],
\end{aligned}
\tag{7}
$$

for $h \in [L]$. The intuition is that $\left[\boldsymbol{f}^{(h+1)}(\boldsymbol{x}) \right]_i = \sum_{j=1}^{d_h} \left[\boldsymbol{W}^{(h+1)} \right]_{i,j} \left[\boldsymbol{g}^{(h)}(\boldsymbol{x}) \right]_j$ is a centered Gaussian process conditioned on $\boldsymbol{f}^{(h)}$ ($\forall i \in [d_{h+1}]$), with covariance

$$
\begin{aligned}
\mathbb{E}\left[\left[\boldsymbol{f}^{(h+1)}(\boldsymbol{x}) \right]_i \cdot \left[\boldsymbol{f}^{(h+1)}(\boldsymbol{x}') \right]_i \bigg| \boldsymbol{f}^{(h)} \right] &= \left\langle \boldsymbol{g}^{(h)}(\boldsymbol{x}), \boldsymbol{g}^{(h)}(\boldsymbol{x}') \right\rangle \\
&= \frac{c_\sigma}{d_h} \sum_{j=1}^{d_h} \sigma\left(\left[\boldsymbol{f}^{(h)}(\boldsymbol{x}) \right]_j \right) \sigma\left(\left[\boldsymbol{f}^{(h)}(\boldsymbol{x}') \right]_j \right),
\end{aligned}
\tag{8}
$$

which converges to $\Sigma^{(h)}(\boldsymbol{x}, \boldsymbol{x}')$ as $d_h \to \infty$ given that each $\left[\boldsymbol{f}^{(h)} \right]_j$ is a centered Gaussian process with covariance $\Sigma^{(h-1)}$. This yields the inductive definition in Equation (7).

3.2   Neural Tangent Kernel

We proceed to derive the NTK for the fully-connected neural net. Recall that we need to compute the value that $\left\langle \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{\theta}}, \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \boldsymbol{\theta}} \right\rangle$ converges to at random initialization in the infinite width limit. We can write the partial derivative with respect to a particular weight matrix $\boldsymbol{W}^{(h)}$ in a compact form:

$$
\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{W}^{(h)}} = \mathbf{b}^{(h)}(\boldsymbol{x}) \cdot \left(\boldsymbol{g}^{(h-1)}(\boldsymbol{x}) \right)^\top, \qquad h = 1, 2, \ldots, L+1,
$$

where

$$
\mathbf{b}_h(\boldsymbol{x}) = \begin{cases} 1 \in \mathbb{R}, & \text{for } h = L+1, \\ \sqrt{\frac{c_\sigma}{d_h}} \boldsymbol{D}^{(h)}(\boldsymbol{x}) \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b}_{h+1}(\boldsymbol{x}) \in \mathbb{R}^{d_h}, & \text{for } h = 1, \ldots, L, \end{cases}
\tag{9}
$$

$$
\boldsymbol{D}^{(h)}(\boldsymbol{x}) = \text{diag}\left(\dot{\sigma}\left(\boldsymbol{f}^{(h)}(\boldsymbol{x}) \right) \right) \in \mathbb{R}^{d_h \times d_h}, \qquad h = 1, \ldots, L.
\tag{10}
$$

Then, for any $h \in [L+1]$, we can compute

$$
\begin{aligned}
\left\langle \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{W}^{(h)}}, \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \boldsymbol{W}^{(h)}} \right\rangle &= \left\langle \mathbf{b}^{(h)}(\boldsymbol{x}) \cdot \left(\boldsymbol{g}^{(h-1)}(\boldsymbol{x}) \right)^\top, \mathbf{b}^{(h)}(\boldsymbol{x}') \cdot \left(\boldsymbol{g}^{(h-1)}(\boldsymbol{x}') \right)^\top \right\rangle \\
&= \left\langle \boldsymbol{g}^{(h-1)}(\boldsymbol{x}), \boldsymbol{g}^{(h-1)}(\boldsymbol{x}') \right\rangle \cdot \left\langle \mathbf{b}^{(h)}(\boldsymbol{x}), \mathbf{b}^{(h)}(\boldsymbol{x}') \right\rangle.
\end{aligned}
$$

Note that we have established in Equation (8) that

$$
\left\langle \boldsymbol{g}^{(h-1)}(\boldsymbol{x}), \boldsymbol{g}^{(h-1)}(\boldsymbol{x}') \right\rangle \to \Sigma^{(h-1)}\left(\boldsymbol{x}, \boldsymbol{x}' \right).
$$

For the other factor $\left\langle \mathbf{b}^{(h)}(\boldsymbol{x}), \mathbf{b}^{(h)}(\boldsymbol{x}') \right\rangle$, by definition (9) we get

$$
\begin{aligned}
&\left\langle \mathbf{b}^{(h)}(\boldsymbol{x}), \mathbf{b}^{(h)}(\boldsymbol{x}') \right\rangle \\
&= \frac{c_\sigma^{L-h}}{d_{h+1}\cdots d_L} \left\langle \sqrt{\frac{c_\sigma}{d_h}} \boldsymbol{D}^{(h)}(\boldsymbol{x}) \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}_{h+1}(\boldsymbol{x}), \sqrt{\frac{c_\sigma}{d_h}} \boldsymbol{D}^{(h)}(\boldsymbol{x}') \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}_{h+1}(\boldsymbol{x}') \right\rangle .
\end{aligned}
\tag{11}
$$

Although $\boldsymbol{W}^{(h+1)}$ and $\mathbf{b}_{h+1}(\boldsymbol{x})$ are dependent, the Gaussian initialization of $\boldsymbol{W}^{(h+1)}$ allows us to replace $\boldsymbol{W}^{(h+1)}$ with a fresh new sample $\widetilde{\boldsymbol{W}}^{(h+1)}$ without changing its limit. This is made rigorous for ReLU activation in Theorem 3.1.

$$
\begin{aligned}
&\left\langle \sqrt{\frac{c_\sigma}{d_h}} \boldsymbol{D}^{(h)}(\boldsymbol{x}) \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}_{h+1}(\boldsymbol{x}), \sqrt{\frac{c_\sigma}{d_h}} \boldsymbol{D}^{(h)}(\boldsymbol{x}') \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}_{h+1}(\boldsymbol{x}') \right\rangle \\
&\approx \left\langle \sqrt{\frac{c_\sigma}{d_h}} \boldsymbol{D}^{(h)}(\boldsymbol{x}) \left(\widetilde{\boldsymbol{W}}^{(h+1)}\right)^\top \mathbf{b}_{h+1}(\boldsymbol{x}), \sqrt{\frac{c_\sigma}{d_h}} \boldsymbol{D}^{(h)}(\boldsymbol{x}') \left(\widetilde{\boldsymbol{W}}^{(h+1)}\right)^\top \mathbf{b}_{h+1}(\boldsymbol{x}') \right\rangle \\
&\to \frac{c_\sigma}{d_h} \operatorname{tr}\left(\boldsymbol{D}^{(h)}(\boldsymbol{x})\boldsymbol{D}^{(h)}(\boldsymbol{x}')\right) \left\langle \mathbf{b}^{(h+1)}(\boldsymbol{x}), \mathbf{b}^{(h+1)}(\boldsymbol{x}') \right\rangle \\
&\to \dot{\Sigma}^{(h)}\left(\boldsymbol{x}, \boldsymbol{x}'\right) \left\langle \mathbf{b}^{(h+1)}(\boldsymbol{x}), \mathbf{b}^{(h+1)}(\boldsymbol{x}') \right\rangle ,
\end{aligned}
$$

where

$$
\dot{\Sigma}^{(h)}(\boldsymbol{x}, \boldsymbol{x}') = c_\sigma \mathop{\mathbb{E}}_{(u,v)\sim\mathcal{N}\left(\mathbf{0},\boldsymbol{\Lambda}^{(h)}\right)} [\dot{\sigma}(u)\dot{\sigma}(v)] .
\tag{12}
$$

Applying this approximation inductively in Equation (11), we get

$$
\left\langle \mathbf{b}^{(h)}(\boldsymbol{x}), \mathbf{b}^{(h)}(\boldsymbol{x}') \right\rangle \to \prod_{h'=h}^{L} \dot{\Sigma}^{(h')}(\boldsymbol{x}, \boldsymbol{x}').
$$

Finally, since $\left\langle \frac{\partial f(\boldsymbol{\theta},\boldsymbol{x})}{\partial \boldsymbol{\theta}}, \frac{\partial f(\boldsymbol{\theta},\boldsymbol{x}')}{\partial \boldsymbol{\theta}} \right\rangle = \sum_{h=1}^{L+1} \left\langle \frac{\partial f(\boldsymbol{\theta},\boldsymbol{x})}{\partial \boldsymbol{W}^{(h)}}, \frac{\partial f(\boldsymbol{\theta},\boldsymbol{x}')}{\partial \boldsymbol{W}^{(h)}} \right\rangle$, we obtain the final NTK expression for the fully-connected neural network:

$$
\Theta^{(L)}(\boldsymbol{x}, \boldsymbol{x}') = \sum_{h=1}^{L+1} \left(\Sigma^{(h-1)}(\boldsymbol{x}, \boldsymbol{x}') \cdot \prod_{h'=h}^{L+1} \dot{\Sigma}^{(h')}(\boldsymbol{x}, \boldsymbol{x}') \right) ,
\tag{13}
$$

where we let $\dot{\Sigma}^{(L+1)}(\boldsymbol{x}, \boldsymbol{x}') = 1$ for convenience.

Rigorously, for ReLU activation, we have the following theorem that gives a concrete bound on the hidden widths that is sufficient for convergence to the NTK at initialization:

Theorem 3.1 (Convergence to the NTK at initializatoin). *Fix $\epsilon > 0$ and $\delta \in (0,1)$. Suppose $\sigma(z) = \max(0, z)$ $(z \in \mathbb{R})$, $\min_{h\in[L]} d_h \geq \operatorname{poly}(L, 1/\epsilon) \cdot \log(L/\delta)$, and $[\boldsymbol{W}^{(h)}]_{i,j} \overset{i.i.d.}{\sim} \mathcal{N}(0,1)$, $\forall h \in [L+1], i \in [d_h], j \in [d_{h-1}]$. Then for any inputs $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^{d_0}$ such that $\|\boldsymbol{x}\| \leq 1, \|\boldsymbol{x}'\| \leq 1$, with probability at least $1 - \delta$ we have:*

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

The proof of Theorem 3.1 is given in Appendix B.

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Remark 3.1. *Theorem 3.1 improves upon previous results [Jacot et al., 2018, Yang, 2019] that establish convergence to the NTK at initialization in the following sense:*

1. *Previous results are asymptotic, i.e., they require the widths to go to infinity, while Theorem 3.1 gives a non-asymptotic bound on the required layer widths.*

2. *Jacot et al. [2018] required sequential limit, i.e., $d_1, \ldots, d_L$ go to infinity one by one, and Yang [2019] let $d_1, \ldots, d_L$ go to infinity at the same rate. On the other hand, Theorem 3.1 only requires $\min_{h \in [L]} d_h$ to be sufficiently large, which is the weakest notion of limit.*

Equivalence between Wide Neural Net and Kernel Regression using NTK. Built on Theorem 3.1, we can further incorporate the training process and show the equivalence between a fully-trained sufficiently wide neural net and the kernel regression solution using the NTK, as described in Lemma 3.1 and the discussion after it.

Recall that the training data are $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \subset \mathbb{R}^d \times \mathbb{R}$, and $\boldsymbol{H}^* \in \mathbb{R}^{n \times n}$ is the NTK evaluated on these training data, i.e., $[\boldsymbol{H}^*]_{i,j} = \Theta^{(L)}(\boldsymbol{x}_i, \boldsymbol{x}_j)$. Denote $\lambda_0 = \lambda_{\min}(\boldsymbol{H}^*)$. For a testing point $\boldsymbol{x}_{te} \in \mathbb{R}^d$, we let $\ker_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{X}) \in \mathbb{R}^n$ be the kernel values of this testing point and n training points, i.e., $[\ker_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{X})]_i = \Theta^{(L)}(\boldsymbol{x}_{te}, \boldsymbol{x}_i)$. The prediction of kernel regression using NTK on this testing point is

$$f_{ntk}(\boldsymbol{x}_{te}) = (\ker_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{X}))^\top (\boldsymbol{H}^*)^{-1} \boldsymbol{y}.$$

Since the above solution corresponds to the linear dynamics in Equation (4) with zero initialization, in order to establish equivalence between neural network and kernel regression, we would like the initial output of the neural network to be small. Therefore, we apply a small multiplier κ, and let the final output of the neural network be

$$f_{nn}(\boldsymbol{\theta}, \boldsymbol{x}) = \kappa f(\boldsymbol{\theta}, \boldsymbol{x}).$$

We let $f_{nn}(\boldsymbol{x}_{te}) = \lim_{t \to \infty} f_{nn}(\boldsymbol{\theta}(t), \boldsymbol{x}_{te})$ be the prediction of the neural network at the end of training.

The following theorem establishes the equivalence between the fully-trained wide neural network f_{nn} and the kernel regression predictor f_{ntk} using the NTK.

Theorem 3.2 (Main theorem). *Suppose $\sigma(z) = \max(0, z)$ ($z \in \mathbb{R}$), $1/\kappa = \text{poly}(1/\epsilon, \log(n/\delta))$ and $d_1 = d_2 = \cdots = d_L = m$ with $m \geq \text{poly}(1/\kappa, L, 1/\lambda_0, n, \log(1/\delta))$. Then for any $\boldsymbol{x}_{te} \in \mathbb{R}^d$ with $\|\boldsymbol{x}_{te}\| = 1$, with probability at least $1 - \delta$ over the random initialization, we have*

$$|f_{nn}(\boldsymbol{x}_{te}) - f_{ntk}(\boldsymbol{x}_{te})| \leq \epsilon.$$

Several comments are in sequel. Theorem 3.2 is, to our knowledge, the first result that rigorously shows the equivalence between a fully-trained neural net and a kernel predictor. Comparing with [Jacot et al., 2018], our bound is non-asymptotic whereas [Jacot et al., 2018] only has an asymptotic result; furthermore, Jacot et al. [2018] required the width of every layer to go to infinity in a sequential order, while we can have the same number of neurons per layer, which is closer to practice. Comparing with recent results on over-parameterized neural nets [Arora et al., 2019, Allen-Zhu et al., 2018b,a, Du et al., 2019, 2018b, Li and Liang, 2018, Zou et al., 2018], our theorem is a more precise characterization of the learned neural network. That is, the prediction is essentially

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a kernel predictor. Therefore, to study the properties of these over-parameterized nets, such as their generalization power, it is sufficient to study the corresponding NTK.

While this theorem only gives guarantee for a single point, using a union bound, we can show that this guarantee holds for (exponentially many) finite testing points. Combing this with the standard analysis of hold-out validation set, we can conclude that a fully-trained wide neural net enjoys the same generalization ability as its corresponding NTK.

For the proof of Theorem 3.2, we first use a generic argument to show that the perturbation on the prediction can be reduced to the perturbation on kernel value at the initialization and during training. Theorem 3.1 guarantees a small perturbation on kernel value at initialization. For the perturbation during training, we use high level proof idea from Du et al. [2018b], Arora et al. [2019] to reduce the perturbation on the kernel value to the perturbation on the gradient of each prediction with respect to weight matrices. Then we adopt technical lemmas from Allen-Zhu et al. [2018b] to obtain bounds on the perturbation of the gradient. See Appendix D for details. We remark that Jacot et al. [2018], Lee et al. [2019] provided proofs for the training part. However, both are asymptotic results and only apply to *finite* training time. In contrast, we give a finite-width perturbation bound and our result applies to *infinite* training time.

4   Convolutional Neural Tangent Kernel

In this section we study convolutional neural networks (CNNs) and their corresponding CNTKs. We study two architectures, vanilla CNN and CNN with global average pooling (GAP). To formally define CNNs, we first introduce some notations. Throughout the paper, we let P be the width and Q be the height of the image. We use $q \in \mathbb{Z}_+$ to denote the filter size. In practice, $q = 1, 3,$ or 5. We use standard zero padding and set stride size to be 1 to make sure the input of each layer has the same size. For a convolutional filter $\boldsymbol{w} \in \mathbb{R}^{q \times q}$ and an image $\boldsymbol{x} \in \mathbb{R}^{P \times Q}$, the convolution operator is defined as

$$[\boldsymbol{w} * \boldsymbol{x}]_{ij} = \sum_{a=-\frac{q-1}{2}}^{\frac{q-1}{2}} \sum_{b=-\frac{q-1}{2}}^{\frac{q-1}{2}} [\boldsymbol{w}]_{a+\frac{q+1}{2}, b+\frac{q+1}{2}} [\boldsymbol{x}]_{a+i, b+j} \text{ for } i \in [P], j \in [Q]. \tag{14}$$

Equation (14) shows patch $[\boldsymbol{w} * \boldsymbol{x}]_{ij}$ depends on $[\boldsymbol{x}]_{i-\frac{q-1}{2}:i+\frac{q-1}{2}, j-\frac{q-1}{2}:j+\frac{q-1}{2}}$. Our CNTK formula also relies on this dependency. For $(i, j, i', j') \in [P] \times [Q] \times [P] \times [Q]$, define

$$\mathcal{D}_{ij,i'j'} = \left\{ (i+a, j+b, i'+a', j'+b') \in [P] \times [Q] \times [P] \times [Q] \mid -(q-1)/2 \le a, b, a', b' \le (q-1)/2 \right\}.$$

Lastly, for a tensor $\boldsymbol{T} \in \mathbb{R}^{P \times Q \times P \times Q}$, we denote $[\boldsymbol{T}]_{\mathcal{D}_{ij,i'j'}} \in \mathbb{R}^{q \times q \times q \times q}$ a sub-tensor and we let $\mathrm{tr}(\boldsymbol{T}) = \sum_{i,j} \boldsymbol{T}_{ij,ij}$.

4.1   Vanilla CNN

The first type of CNN is the vanilla CNN which consists L convolution layers and one fully-connected layer, formally defined as follows.

CNN Definition

- Let $\boldsymbol{x}^{(0)} = \boldsymbol{x} \in \mathbb{R}^{P \times Q \times C^{(0)}}$ be the input image where $C^{(0)}$ is the number of channels in the input image.

- For $h = 1, \ldots, L$, $\beta = 1, \ldots, C^{(h)}$, the intermediate outputs are defined as

$$\tilde{\boldsymbol{x}}_{(\beta)}^{(h)} = \sum_{\alpha=1}^{C^{(h-1)}} \boldsymbol{W}_{(\alpha),(\beta)}^{(h)} * \boldsymbol{x}_{(\alpha)}^{(h-1)}, \quad \boldsymbol{x}_{(\beta)}^{(h)} = \sqrt{\frac{c_\sigma}{C^{(h)} \times q \times q}} \sigma\left(\tilde{\boldsymbol{x}}_{(\beta)}^{(h)}\right)$$

where each $\boldsymbol{W}_{(\alpha),(\beta)}^{(h)} \in \mathbb{R}^{q \times q}$ is a filter with Gaussian initialization.

- The final output is defined as

$$f(\boldsymbol{\theta}, \boldsymbol{x}) = \sum_{\alpha=1}^{C^{(L)}} \left\langle \boldsymbol{W}_{(\alpha)}^{(L+1)}, \boldsymbol{x}_{(\alpha)}^{(L)} \right\rangle$$

where $\boldsymbol{W}_{(\alpha)}^{(L+1)} \in \mathbb{R}^{P \times Q}$ is a weight matrix with Gaussian initialization.

For this architecture, using the same reasoning as in Section 3.2, we obtain the following convolutional neural tangent kernel formula. The details are provided in Appendix E. We will use a dynamic programming approach to compute the kernel.

CNTK Formula. We let $\boldsymbol{x}, \boldsymbol{x}'$ be two input images.

- For $\alpha = 1, \ldots, C^{(0)}$, $(i, j, i', j') \in [P] \times [Q] \times [P] \times [Q]$, define

$$\boldsymbol{K}_{(\alpha)}^{(0)}\left(\boldsymbol{x}, \boldsymbol{x}'\right) = \boldsymbol{x}_{(\alpha)} \otimes \boldsymbol{x}'_{(\alpha)} \text{ and } \left[\boldsymbol{\Sigma}^{(0)}(\boldsymbol{x}, \boldsymbol{x}')\right]_{ij,i'j'} = \sum_{\alpha=1}^{C^{(0)}} \operatorname{tr}\left(\left[\boldsymbol{K}_{(\alpha)}^{(0)}(\boldsymbol{x}, \boldsymbol{x}')\right]_{\mathcal{D}_{ij,i'j'}}\right).$$

- For $h \in [L]$,

  - For $(i, j, i', j') \in [P] \times [Q] \times [P] \times [Q]$, define

$$\boldsymbol{\Lambda}_{ij,i'j'}^{(h)}(\boldsymbol{x}, \boldsymbol{x}') = \begin{pmatrix} \left[\boldsymbol{\Sigma}^{(h-1)}(\boldsymbol{x}, \boldsymbol{x})\right]_{ij,ij} & \left[\boldsymbol{\Sigma}^{(h-1)}(\boldsymbol{x}, \boldsymbol{x}')\right]_{ij,i'j'} \\ \left[\boldsymbol{\Sigma}^{(h-1)}\left(\boldsymbol{x}', \boldsymbol{x}\right)\right]_{i'j',ij} & \left[\boldsymbol{\Sigma}^{(h-1)}\left(\boldsymbol{x}', \boldsymbol{x}'\right)\right]_{i'j',i'j'} \end{pmatrix} \in \mathbb{R}^{2 \times 2}.$$

  - Define $\boldsymbol{K}^{(h)}(\boldsymbol{x}, \boldsymbol{x}'), \dot{\boldsymbol{K}}^{(h)}(\boldsymbol{x}, \boldsymbol{x}') \in \mathbb{R}^{P \times Q \times P \times Q}$, for $(i, j, i', j') \in [P] \times [Q] \times [P] \times [Q]$

$$\left[\boldsymbol{K}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right]_{ij,i'j'} = \mathop{\mathbb{E}}_{(u,v) \sim \mathcal{N}\left(\mathbf{0}, \boldsymbol{\Lambda}_{ij,i'j'}^{(h)}(\boldsymbol{x},\boldsymbol{x}')\right)} \left[\sigma\left(u\right)\sigma\left(v\right)\right], \tag{15}$$

$$\left[\dot{\boldsymbol{K}}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right]_{ij,i'j'} = \mathop{\mathbb{E}}_{(u,v) \sim \mathcal{N}\left(\mathbf{0}, \boldsymbol{\Lambda}_{ij,i'j'}^{(h)}(\boldsymbol{x},\boldsymbol{x}')\right)} \left[\dot{\sigma}\left(u\right)\dot{\sigma}\left(v\right)\right]. \tag{16}$$

  - Define $\boldsymbol{\Sigma}^{(h)}(\boldsymbol{x}, \boldsymbol{x}') \in \mathbb{R}^{P \times Q \times P \times Q}$, for $(i, j, i', j') \in [P] \times [Q] \times [P] \times [Q]$

$$\left[\boldsymbol{\Sigma}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right]_{ij,i'j'} = \frac{c_\sigma}{q^2} \operatorname{tr}\left(\left[\boldsymbol{K}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right]_{\mathcal{D}_{ij,i'j'}}\right).$$

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Note that $\mathbf{\Sigma}(\boldsymbol{x}, \boldsymbol{x}')$ and $\dot{\mathbf{\Sigma}}(\boldsymbol{x}, \boldsymbol{x}')$ share similar structures as their NTK counterparts. The only difference is that we have one more step, taking the trace over patches. This step represents the convolution operation in the corresponding CNN. Next, we can use a recursion to compute the final kernel value.

1. First, we define $\mathbf{\Theta}^{(0)}(\boldsymbol{x}, \boldsymbol{x}') = \mathbf{\Sigma}^{(0)}(\boldsymbol{x}, \boldsymbol{x}')$.

2. For $h = 1, \ldots, L$ and $(i, j, i', j') \in [P] \times [Q] \times [P] \times [Q]$, we define

$$\left[\mathbf{\Theta}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right]_{ij,i'j'} = \frac{c_\sigma}{q^2} \mathrm{tr}\left(\left[\dot{\boldsymbol{K}}^{(h)}(\boldsymbol{x}, \boldsymbol{x}') \odot \mathbf{\Theta}^{(h-1)}(\boldsymbol{x}, \boldsymbol{x}') + \boldsymbol{K}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right]_{D_{ij,i'j'}}\right).$$

3. Lastly, the final kernel value is defined as

$$\mathrm{tr}\left(\mathbf{\Theta}^{(L)}(\boldsymbol{x}, \boldsymbol{x}')\right).$$

4.2   CNN with Global Average Pooling

We also consider another architecture, CNN with global average pooling.

CNN Definition

- Let $\boldsymbol{x} = \boldsymbol{x}^{(0)} \in \mathbb{R}^{P \times Q \times C^{(0)}}$ be the input image and $C^{(0)}$ is the number of initial channels.

- For $h = 1, \ldots, L$, $\beta = 1, \ldots, C^{(h)}$, the intermediate outputs are defined as

$$\tilde{\boldsymbol{x}}^{(h)}_{(\beta)} = \sum_{\alpha=1}^{C^{(h-1)}} \boldsymbol{W}^{(h)}_{(\alpha),(\beta)} * \boldsymbol{x}^{(h-1)}_{(\alpha)}, \quad \boldsymbol{x}^{(h)}_{(\beta)} = \sqrt{\frac{c_\sigma}{C^{(h)} \times q^{(h)} \times q^{(h)}}} \sigma\left(\tilde{\boldsymbol{x}}^{(h)}_{(\beta)}\right).$$

- The final output is defined as

$$f(\boldsymbol{\theta}, \boldsymbol{x}) = \sum_{\alpha=1}^{C^{(L)}} W^{(L+1)}_{(\alpha)} \left(\frac{1}{PQ} \sum_{(i,j) \in [P] \times [Q]} \left[\boldsymbol{x}^{(L)}_{(\alpha)}\right]_{ij}\right).$$

where $W^{(L+1)}_{(\alpha)} \in \mathbb{R}$ is a scalar with Gaussian initialization.

Besides using global average pooling, another modification is that we do not train the first and the layer. This is inspired by Du et al. [2018a] in which authors showed that if one applies gradient flow, then at any training time t, the difference between the squared Frobenius norm of the weight matrix at time t and that at initialization is same for all layers. However, note that $\boldsymbol{W}^{(1)}$ and $\boldsymbol{W}^{(L+1)}$ are special because they are smaller matrices compared with other intermediate weight matrices, so *relatively*, these two weight matrices change more than the intermediate matrices during the training process, and this may dramatically change the kernel. Therefore, we choose to fix $\boldsymbol{W}^{(1)}$ and $\boldsymbol{W}^{(L+1)}$ to the make over-parameterization theory closer to practice.

CNTK Formula. We let x, x' be two input images. Note because CNN with global average pooling and vanilla CNN shares the same architecture except the last layer, $\mathbf{\Sigma}^{(h)}(x, x')$, $\dot{\mathbf{\Sigma}}^{(h)}(x, x')$ and $K^{(h)}(x, x')$ are the same for these two architectures. the only difference is in calculating the final kernel value. To compute the final kernel value, we use the following procedure.

1. First, we define $\mathbf{\Theta}^{(0)}(x, x') = \mathbf{0}$. Note this is different from CNTK for vanilla CNN which uses $\mathbf{\Sigma}^{(0)}$ as the initial value because we do not train the first layer.

2. For $h = 1, \ldots, L - 1$ and $(i, j, i', j') \in [P] \times [Q] \times [P] \times [Q]$, we define

$$\left[\mathbf{\Theta}^{(h)}(x, x') \right]_{ij,i'j'} = \frac{c_\sigma}{q^2} \operatorname{tr} \left(\left[\dot{K}^{(h)}(x, x') \odot \mathbf{\Theta}^{(h-1)}(x, x') + K^{(h)}(x, x') \right]_{D_{ij,i'j'}} \right).$$

3. For $(i, j, i', j') \in [P] \times [Q] \times [P] \times [Q]$, we define

$$\left[\mathbf{\Theta}^{(L)}(x, x') \right]_{ij,i'j'} = \frac{c_\sigma}{q^2} \operatorname{tr} \left(\left[\dot{K}^{(L)}(x, x') \odot \mathbf{\Theta}^{(L-1)}(x, x') \right]_{D_{ij,i'j'}} \right).$$

4. Lastly, the final kernel value is defined as

$$\frac{1}{P^2 Q^2} \sum_{(i,j,i',j') \in [P] \times [Q] \times [P] \times [Q]} \left[\mathbf{\Theta}^{(L)}(x, x') \right]_{ij,i'j'}.$$

Note that we ignore $K^{(L)}$ comparing with the CNTK of CNN. This is because we do not train the last layer. The other difference is we calculate the mean over all entries, instead of calculating the summation over the diagonal ones. This is because we use global average pooling so the cross-variances between every two patches will contribute to the kernel.

4.3 Fast Computation for ReLU-Activated CNTK

To compute the CNTK corresponding to a CNN with L convolution layers and one fully-connected layer on n samples, the time complexity is $O(n^2 P^2 Q^2 \cdot L)$. Previous work assumed that directly computing convolutional kernel exactly is computationally infeasible, and thus resorted to approximations like Monte Carlo sampling [Novak et al., 2019]. In this section, we present a new approach to efficiently compute CNTK for ReLU activation *exactly*. Most computation required by our new approach can be described as entry-wise operations over matrices and tensors, which allows efficient implementations on GPUs.

Following the formulas in Sections 4.1 and 4.2, the trickiest part is computing the expectation of the post-activation output, i.e., Equation (15) and (16). These two expectations depend on (the same) 2×2 matrices $\left[\mathbf{\Lambda}^{(h)}(x, x') \right]_{ij,i'j'}$. To obtain faster implementations, our key observation is that if the diagonal entries of $\left[\mathbf{\Lambda}^{(h)}(x, x') \right]_{ij,i'j'}$ are all ones and the activation function is ReLU, there are closed-form formulas for the the corresponding expectations. To see this, let us suppose for now that $\mathbf{\Lambda} = \begin{pmatrix} 1 & \lambda \\ \lambda & 1 \end{pmatrix}$ for some $|\lambda| \leq 1$. When the activation function $\sigma(\cdot)$ is ReLU, one can show that

$$\mathbb{E}_{(u,v) \sim \mathcal{N}(\mathbf{0}, \mathbf{\Lambda})} \left[\sigma(u) \sigma(v) \right] = \frac{\lambda(\pi - \arccos(\lambda)) + \sqrt{1 - \lambda^2}}{2\pi} \tag{17}$$

and

$$\mathop{\mathbb{E}}_{(u,v)\sim\mathcal{N}(\mathbf{0},\mathbf{\Lambda})}\left[\dot{\sigma}\left(u\right)\dot{\sigma}\left(v\right)\right]=\frac{\pi-\arccos\left(\lambda\right)}{2\pi}. \tag{18}$$

Now we let

$$\boldsymbol{A}^{(h)}=\begin{pmatrix}\boldsymbol{\Sigma}^{(h-1)}(\boldsymbol{x},\boldsymbol{x}) & \boldsymbol{\Sigma}^{(h-1)}(\boldsymbol{x},\boldsymbol{x}') \\ \boldsymbol{\Sigma}^{(h-1)}\left(\boldsymbol{x}',\boldsymbol{x}\right) & \boldsymbol{\Sigma}^{(h-1)}\left(\boldsymbol{x}',\boldsymbol{x}'\right)\end{pmatrix}\in\mathbb{R}^{2PQ\times2PQ}.$$

Here, we interpret $\boldsymbol{\Sigma}^{(h-1)}(\boldsymbol{x},\boldsymbol{x})$, $\boldsymbol{\Sigma}^{(h-1)}(\boldsymbol{x},\boldsymbol{x}')$, $\boldsymbol{\Sigma}^{(h-1)}\left(\boldsymbol{x}',\boldsymbol{x}\right)$ and $\boldsymbol{\Sigma}^{(h-1)}\left(\boldsymbol{x}',\boldsymbol{x}'\right)$ as matrices of size $PQ\times PQ$. If the diagonal entries of $A^{(h)}$ are all ones, then the diagonal entries of $\left[\boldsymbol{\Lambda}^{(h)}(\boldsymbol{x},\boldsymbol{x}')\right]_{ij,i'j'}$ are all ones for all possible $(i,j,i',j')\in[P]\times[Q]\times[P]\times[Q]$, in which case we can calculate $\boldsymbol{K}^{(h)}(\boldsymbol{x},\boldsymbol{x}')$ and $\dot{\boldsymbol{K}}^{(h)}(\boldsymbol{x},\boldsymbol{x}')$ by simply applying the closed-form formulas described in (17) and (18) on $A^{(h)}$.

However, in general, the diagonal entries of $\boldsymbol{A}^{(h)}$ are not always all ones, in which case we resort to the homogeneity of the ReLU activation function. Suppose $\boldsymbol{\Lambda}=\begin{pmatrix}1 & \lambda \\ \lambda & 1\end{pmatrix}$ for some $|\lambda|\leq1$, and $\boldsymbol{D}=\begin{pmatrix}c_1 & 0 \\ 0 & c_2\end{pmatrix}$ for some $c_1,c_2\geq0$, then one can show that

$$\mathop{\mathbb{E}}_{(u,v)\sim\mathcal{N}(\mathbf{0},\boldsymbol{D\Lambda D})}\left[\sigma\left(u\right)\sigma\left(v\right)\right]=\frac{\lambda(\pi-\arccos(\lambda))+\sqrt{1-\lambda^2}}{2\pi}\cdot c_1c_2 \tag{19}$$

and

$$\mathop{\mathbb{E}}_{(u,v)\sim\mathcal{N}(\mathbf{0},\boldsymbol{D\Lambda D})}\left[\dot{\sigma}\left(u\right)\dot{\sigma}\left(v\right)\right]=\frac{\pi-\arccos\left(\lambda\right)}{2\pi}. \tag{20}$$

Inspired by this, our final approach is described as follows.

1. Let $\boldsymbol{D}=\begin{pmatrix}\boldsymbol{D_x} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{D_{x'}}\end{pmatrix}$, where $\boldsymbol{D_x}$ and $\boldsymbol{D_{x'}}$ are diagonal matrices whose diagonal entries are square roots of the diagonal entries of $\boldsymbol{\Sigma}^{(h-1)}(\boldsymbol{x},\boldsymbol{x})$ and $\boldsymbol{\Sigma}^{(h-1)}(\boldsymbol{x'},\boldsymbol{x'})$, respectively.

2. Applying Equations (19) and (20) on $\boldsymbol{A}^{(h)}=\boldsymbol{D\Lambda}^{(h)}\boldsymbol{D}$, where the diagonal entries of $\boldsymbol{\Lambda}^{(h)}$ are all ones.

Notice that the implementation above requires us to store the whole $\boldsymbol{A}^{(h)}$ matrix, which has size $2PQ\times2PQ$. To further optimize the efficiency, we notice that to implement the approach described above, we only need to store the diagonal entries of $\boldsymbol{\Sigma}^{(h-1)}(\boldsymbol{x},\boldsymbol{x})$ and $\boldsymbol{\Sigma}^{(h-1)}(\boldsymbol{x'},\boldsymbol{x'})$, together with the matrix $\boldsymbol{\Sigma}^{(h-1)}(\boldsymbol{x},\boldsymbol{x'})$, which has size $PQ\times PQ$.

5 Experiments

In this section, we present our empirical findings. In Section 5.1, we compare the performances between CNNs and their corresponding CNTKs on CIFAR-10 dataset. In Section 5.2, we compare the performances between CNTKs and their corresponding random features on CIFAR-2 dataset.

Depth	CNN-V	CNTK-V	CNTK-V-2K	CNN-GAP	CNTK-GAP	CNTK-GAP-2K
3	61.97%	64.47%	40.94%	57.96%	70.47%	49.71%
4	62.12%	65.52%	42.54%	80.58%	75.93%	51.06%
6	64.03%	66.03%	43.43%	80.97%	76.73%	51.73%
11	70.97%	65.90%	43.42%	75.45%	77.43%	51.92%
21	80.56%	64.09%	42.53%	81.23%	77.08%	52.22%

Table 1: Classification accuracies of CNNs and CNTKs on the CIFAR-10 dataset. CNN-V represents vanilla CNN and CNTK-V represents the kernel corresponding to CNN-V. CNN-GAP represents CNN with GAP and CNTK-GAP represents the kernel correspondong to CNN-GAP. CNTK-V-2K and CNTK-GAP-2K represent training CNTKs with only 2,000 training data.

5.1   Performance of CNTK

Setup.   Due to efficiency considerations, for all experiments, we use no data augmentation. Tricks like Batch Normalization, Dropout, Weight Decay, etc. are not used for proper comparison. We fix the filter q to be 3 and stride to be 1. We use zero padding to make sure the number of patches keeps unchanged after each convolutional layer. We set the number of convolution layers to be 2, 3, 5, 10, or 20. For both CNNs and CNTKs, we use the quadratic loss as the objective function.

Following Novak et al. [2019], for a label $c \in \{1, \ldots, 10\}$, we use $-0.1 \cdot \mathbf{1} + \mathbf{e}_c$ as its encoding. For example, if the class label is 3, we use $(-0.1, -0.1, 0.9, -0.1, \ldots, -0.1)$ as its encoding. During training time, we calculate $(\mathbf{H}^*)^{-1}\mathbf{Y}$, where $\mathbf{H}^*$ is the CNTK kernel matrix, and the i-th row of $\mathbf{Y} \in \mathbb{R}^{n \times 10}$ is the encoding of the label of the i-th data. During testing time, for a test data point $\mathbf{x}_{te}$, we calculate

$$f^*(\mathbf{x}_{te}) = (\ker(\mathbf{x}_{te}, \mathbf{x}_1), \ldots, \ker(\mathbf{x}_{te}, \mathbf{x}_n)) \cdot (\mathbf{H}^*)^{-1}\mathbf{Y}$$

and choose the class with largest value as the prediction.

The architecture of CNNs is as described in Section 4. To train CNNs, we use stochastic gradient descent (SGD) with different learning rates, different number of channels in the convolution layers and different values for κ. The learning rate is fixed throughout the training process. For CNNs, we report the best performance among all hyperparameters.

Our neural networks are trained using the PyTorch package, using (possibly multiple) NVIDIA Tesla V100 GPUs. We calculate the kernel values using the CuPy[3] package. For time-consuming operations, we write native CUDA codes to speed up the calculation. All experiments are performed on Amazon Web Services (AWS).

Main Results.   We test two different types of architectures, vanilla CNN and CNN with global average pooling (GAP) with fixed first and last layer as described in Section 4. We also test CNTKs with only 2,000 training data to see whether their performances are consistent with CNTKs and CNNs using the full training set. The results are summarized in Table 1. Notice that in Table 1, depth is the total number of layers (including both convolution layers and fully-connected layers).

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[3] https://cupy.chainer.org.

Several comments are in sequel. First, CNTKs are very powerful kernels. The best kernel, 11-layer CNTK with GAP, achieves 77.43% classification accuracy on CIFAR-10. This results in a significant new benchmark for performance of a pure kernel-based method on CIFAR-10, being 10% higher than methods reported in [Novak et al., 2019].

Second, we find that for both CNN and CNTK, depth can affect the classification accuracy. This observation demonstrates that depth not only matters in deep neural networks but can also affect the performance of CNTKs.

Third, the global average pooling operation can significantly increase the classification accuracy by 8% - 10% for both CNN and CNTK. Based on this finding, we expect that many techniques that improve the performance of neural networks are in some sense universal, i.e., these techniques can also benefit kernel methods.

Fourth, we find that there is still a 5% - 6% performance gap between CNTKs and CNNs. Since CNTKs exactly correspond to infinitely wide CNNs, this performance gap implies that finite width has its benefits. Therefore, recent work on over-parameterization [Du et al., 2019, 2018b, Allen-Zhu et al., 2018b,a, Arora et al., 2019, Jacot et al., 2018, Zou et al., 2018] cannot fully explain the success of neural networks yet and we believe it is an interesting open problem to characterize this gap theoretically.

Potential Application in Neural Architecture Search. Finally, we find that performances of CNTK-V-2Ks and CNTK-GAP-2Ks are highly correlated to their CNN-V, CNTK-V, CNN-GAP and CNTK-GAP counterparts. Again we see CNTK-GAP-2Ks outperform CNTK-V-2Ks by a large margin (about 8% - 9%). One potential application of this observation is to guide neural architecture search. We can compute the kernel on a small training data, test it on a validation set, and choose neural network architectures based on the performance of this small kernel on the validation set. We leave large scale experiments of this idea for future work.

5.2 The Importance of Using the Exact Kernel

Now we verify the importance of using the exact kernels instead of the approximated ones from random features (as done in [Lee et al., 2019]). The random features are generated by taking the gradient of the randomly initialized CNNs with respect to the weight matrices. For all CNNs we set the number of channels to be 128. We compare the performances of the exact kernels and the random kernels on the CIFAR-2 dataset, i.e., the first two class in CIFAR-10. For each kernel generated by random features, we test 10 times and report the median. The results are summarized in Table 2. Note that even on the simple CIFAR-2 dataset, random features have much worse accuracies than exact kernels by a large margin. This experiment demonstrates the importance of using the exact kernels instead of the approximated ones.

6 Discussion

This paper gives the first efficient exact algorithm (based upon dynamic programming) for computing CNTK. We also give a rigorous proof that a fully-trained sufficiently wide net is indeed equivalent to the kernel regression predictor using NTK. Below we list some directions for future work.

Depth	RF from Vanilla CNTK	Vanilla CNTK	RF for CNTK-GAP	CNTK-GAP
3	87.25%	92.15%	51.10%	71.05%
4	87.78%	92.80%	52.85%	94.50%
6	88.73%	93.10%	53.98%	95.25%
11	87.80%	93.05%	56.55%	95.40%
21	85.35%	91.95%	90.65%	95.70%

Table 2: Classification accuracies of random kernels generated from random features and exact CNTKs on CIFAR-2.

First, there is a performance gap between CNTKs and CNNs. As we have shown, CNTK has the same prediction as infinitely wide CNN, which means such performance gap must origin from the finite width effect. We believe it is an important theoretical open problem to explain this gap.

Second, empirically, CNTK shows promising results in the image domain. For other domains such as natural language processing and social network analysis, recurrent neural network (RNN) and graph neural network (GNN) are more commonly used. It is an interesting problem to find NTK counterparts of RNNs and GNNs and test their performances.

Third, in this paper, we only "translate" the vanilla CNN and CNN with global average pooling to the corresponding kernels. The state-of-the-art convolutional neural network image classifiers also rely on many other techniques, such as max-pooling, batch-normalization, residual blocks, to name a few. We believe it is possible to "translate" these techniques to kernels as well.

Lastly, the new convolutional kernels are very different from classical Gaussian kernels. Currently, we are not aware of any rigorous theory to explain the generalization behavior of NTKs and CNTKs with multiple layers. Indeed, this can be viewed as another example of our lack of understandings of kernel methods [Belkin et al., 2018]. An immediate open problem is to understand why CNTKs can outperform classical kernels on image classification tasks. As a concrete question, is there any function that can be efficiently learned through CNTKs but not Gaussian kernel? What structural properties of image distributions could explain this supremacy?

Acknowledgments

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A   Proof of Lemma 3.1

Proof of Lemma 3.1. The parameters $\boldsymbol{\theta}$ evolve according to the differential equation

$$\frac{\mathrm{d}\boldsymbol{\theta}(t)}{\mathrm{d}t} = -\nabla\ell(\boldsymbol{\theta}(t)) = -\sum_{i=1}^{n}\left(f(\boldsymbol{\theta}(t),\boldsymbol{x}_i) - y_i\right)\frac{\partial f(\boldsymbol{\theta}(t),\boldsymbol{x}_i)}{\partial\boldsymbol{\theta}}, \tag{21}$$

where $t \geq 0$ is a continuous time index. Under Equation (21), the evolution of the network output $f(\boldsymbol{\theta}(t),\boldsymbol{x}_i)$ can be written as

$$\frac{\mathrm{d}f(\boldsymbol{\theta}(t),\boldsymbol{x}_i)}{\mathrm{d}t} = -\sum_{j=1}^{n}(f(\boldsymbol{\theta}(t),\boldsymbol{x}_j) - y_j)\left\langle \frac{\partial f(\boldsymbol{\theta}(t),\boldsymbol{x}_i)}{\partial\boldsymbol{\theta}}, \frac{\partial f(\boldsymbol{\theta}(t),\boldsymbol{x}_j)}{\partial\boldsymbol{\theta}}\right\rangle, \qquad \forall i \in [n]. \tag{22}$$

Since $\boldsymbol{u}(t) = (f(\boldsymbol{\theta}(t),\boldsymbol{x}_i))_{i\in[n]} \in \mathbb{R}^n$ is the network outputs on all $\boldsymbol{x}_i$'s at time t, and $\boldsymbol{y} = (y_i)_{i\in[n]}$ is the desired outputs, Equation (22) can be written more compactly as

$$\frac{\mathrm{d}\boldsymbol{u}(t)}{\mathrm{d}t} = -\boldsymbol{H}(t)\cdot(\boldsymbol{u}(t) - \boldsymbol{y}), \tag{23}$$

where $\boldsymbol{H}(t) \in \mathbb{R}^{n\times n}$ is a kernel matrix defined as $[\boldsymbol{H}(t)]_{i,j} = \left\langle \frac{\partial f(\boldsymbol{\theta}(t),\boldsymbol{x}_i)}{\partial\boldsymbol{\theta}}, \frac{\partial f(\boldsymbol{\theta}(t),\boldsymbol{x}_j)}{\partial\boldsymbol{\theta}}\right\rangle$ ($\forall i,j \in [n]$). $\qquad\square$

B   Proof of Convergence to NTK at Initialization (Theorem 3.1)

B.1   Notation and some facts about $\sigma(z) = \max(0,z)$

Definition B.1 (*k*-homogeneous function)**.** *A function $f : \mathbb{R} \to \mathbb{R}$ is said to be k-homogeneous, if $f(\lambda x) = \lambda^k f(x)$ for all $x \in \mathbb{R}, \lambda > 0$.*

Definition B.2. *Let $\mathcal{S}^+$ be the set of* positive semi-definite kernels *over $\mathbb{R}^d$, that is*

$$\mathcal{S}^+ = \left\{K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \middle| \forall N \in \mathbb{N}, \boldsymbol{x}_1, \dots \boldsymbol{x}_N \in \mathbb{R}^d, c_1, \dots, c_N \in \mathbb{R}, \ \sum_{i=1}^{N}\sum_{j=1}^{N}c_i c_j K(x_i,x_j) \geq 0. \right\}$$

Let $\sigma : \mathbb{R} \to \mathbb{R}$ be the activation function, and $\mathcal{T}_\sigma : \mathcal{S}^+ \to \mathcal{S}^+$ be the operator induced by σ,

$$\forall \boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^d, \quad \mathcal{T}_\sigma(K)(\boldsymbol{x}, \boldsymbol{x}') = c_\sigma \mathop{\mathbb{E}}_{(u,v)\sim\mathcal{N}\left(\mathbf{0}, \boldsymbol{K}|_{\boldsymbol{x},\boldsymbol{x}'}\right)} \left[\sigma\left(u\right)\sigma\left(v\right)\right],$$

where $\boldsymbol{K}|_{\boldsymbol{x},\boldsymbol{x}'} \in \mathbb{R}^{2\times2}$, $\boldsymbol{K}|_{\boldsymbol{x},\boldsymbol{x}'} = \begin{bmatrix} K(\boldsymbol{x},\boldsymbol{x}) & K(\boldsymbol{x},\boldsymbol{x}') \\ K(\boldsymbol{x}',\boldsymbol{x}) & K(\boldsymbol{x}',\boldsymbol{x}') \end{bmatrix}$.

For convenience, we use $t_\sigma(\boldsymbol{\Sigma})$ to denote $c_\sigma \mathbb{E}_{(u,v)\sim\mathcal{N}(\mathbf{0},\boldsymbol{\Sigma})}\left[\sigma\left(u\right)\sigma\left(v\right)\right]$, and define $\hat{t}_\sigma(\rho)$ as

$$\hat{t}_\sigma(\rho) = c_\sigma \mathop{\mathbb{E}}_{(u,v)\sim\boldsymbol{\Sigma}'}\left[\sigma\left(u\right)\sigma\left(v\right)\right], \text{ with } \boldsymbol{\Sigma}' = \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}$$

When σ is k-homogeneous function, we have

$$t_\sigma(\boldsymbol{\Sigma}) = c_\sigma \left(\Sigma_{11}\Sigma_{22}\right)^{\frac{k}{2}} \mathop{\mathbb{E}}_{(u,v)\sim\mathcal{N}(\mathbf{0},\boldsymbol{\Sigma}')}\left[\sigma\left(u\right)\sigma\left(v\right)\right] \quad \text{with} \quad \boldsymbol{\Sigma}' = \begin{bmatrix} 1 & \frac{\Sigma_{12}}{\sqrt{\Sigma_{11}\Sigma_{22}}} \\ \frac{\Sigma_{12}}{\sqrt{\Sigma_{11}\Sigma_{22}}} & 1 \end{bmatrix}.$$

Thus $t_\sigma(\boldsymbol{\Sigma})$ can be written as $c_\sigma \left(\Sigma_{11}\Sigma_{22}\right)^{\frac{k}{2}} \hat{t}(\frac{\Sigma_{12}}{\sqrt{\Sigma_{11}\Sigma_{22}}})$,

Fact B.1 (Some facts about $\sigma\left(z\right) = \max(0, z)$ and $\mathcal{T}_\sigma$).

1. *For all activation function σ, $t_\sigma\left(\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\right) = 1$.*

2. *For all 1-homogeneous activation σ, $\hat{t}_\sigma(1) = 1$ and $t_\sigma\left(\begin{bmatrix} a & a \\ a & a \end{bmatrix}\right) = a^k$.*

3. *For $\sigma\left(z\right) = \max(0, z)$, $\hat{t}_\sigma(\rho) = \frac{\sqrt{1-\rho^2}+\rho\arcsin\rho}{\pi} + \frac{x}{2}$, $\hat{t}_{\dot{\sigma}}(\rho) = \frac{1}{2} + \frac{\arcsin\rho}{\pi}$ and $c_\sigma = c_{\dot{\sigma}} = 2$.*

Lemma B.1 (Uniform Continuity of $\arcsin z$).

1. *For any $-\frac{\pi}{2} \le y' \le y \le \frac{\pi}{2}$, $\sin y - \sin y' \ge 2\sin^2\frac{y-y'}{2}$.*

2. *$\sin y \ge \frac{2y}{\pi}$, $\forall y \in [0, \frac{\pi}{2}]$.*

3. *$\arcsin$ is uniform continuous: for every $\epsilon \in \mathbb{R}^+$, $|z - z'| < \frac{2\epsilon^2}{\pi^2} \Rightarrow |\arcsin z - \arcsin z'| < \epsilon$.*

4. *For $\sigma\left(z\right) = \max(0, z)$, $\hat{t}_{\dot{\sigma}}$ is uniform continuous: for every $\epsilon \in \mathbb{R}^+$, $|z - z'| < 2\epsilon^2 \Rightarrow |\hat{t}_{\dot{\sigma}}\left(z\right) - \hat{t}_{\dot{\sigma}}\left(z'\right)| < \epsilon$.*

Proof of Lemma B.1. (1). From $-\frac{\pi}{2} \le y' \le y' \le \frac{\pi}{2}$ we know $\frac{-\pi}{2} + \frac{y-y'}{2} \le \frac{y+y'}{2} \le \frac{\pi}{2} - \frac{y-y'}{2}$, which implies that $\cos(\frac{y+y'}{2}) \ge \sin(\frac{y-y'}{2})$. Thus,

$$\sin y \sin y' = 2\cos\frac{y+y'}{2}\sin\frac{y-y'}{2} \ge 2\sin^2\frac{y-y'}{2}.$$

(2). Note that $\left(\frac{\sin y}{y}\right)' = \frac{y\cos y - \sin y}{y^2} = \frac{\cos y}{y^2}(y - \tan y) < 0$, $\frac{\sin y}{y}$ is decreasing on $[0, \frac{\pi}{2}]$. Thus $\frac{\sin y}{y} \ge \frac{1}{\frac{\pi}{2}} = \frac{2}{\pi}$, $\forall y \in [0, \frac{\pi}{2}]$.

(3). Let $y, y' \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, such that $\sin y = z, \sin y' = z'$. W.l.o.g., we assume $y' < y$, $z' < z$. Combing (1) and (2), we have $z - z' = \sin y - \sin y' \ge 2\sin^2\frac{y-y'}{2} \ge \frac{2(y-y')^2}{\pi^2}$. Thus $z - z' \le \frac{2\epsilon^2}{\pi^2} \Longrightarrow$ $\arcsin z - \arcsin z' = y - y' \le \epsilon$. $\square$

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Recall the definition in Equation (7) and (12), we have

$$\Sigma^{(0)}(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{x}^\top \boldsymbol{x}',$$

$$\boldsymbol{\Lambda}^{(h)}(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{\Sigma}^{(h-1)}\Big|_{\boldsymbol{x},\boldsymbol{x}'} = \begin{pmatrix} \Sigma^{(h-1)}(\boldsymbol{x}, \boldsymbol{x}) & \Sigma^{(h-1)}(\boldsymbol{x}, \boldsymbol{x}') \\ \Sigma^{(h-1)}(\boldsymbol{x}', \boldsymbol{x}) & \Sigma^{(h-1)}(\boldsymbol{x}', \boldsymbol{x}') \end{pmatrix} \in \mathbb{R}^{2 \times 2},$$

$$\Sigma^{(h)}(\boldsymbol{x}, \boldsymbol{x}') = c_\sigma \mathop{\mathbb{E}}_{(u,v) \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Lambda}^{(h)})} [\sigma(u)\sigma(v)],$$

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

for $h = 1, \ldots, L$.

For $\sigma(z) = \max(z, 0)$, we have

$$\Sigma^{(h)}(\boldsymbol{x}, \boldsymbol{x}) = \|\boldsymbol{x}\|^2, \quad \forall 0 \leq h \leq L.$$

Let $\boldsymbol{D} = \boldsymbol{D}(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{D}^{(h)}(\boldsymbol{x})\boldsymbol{D}^{(h)}(\boldsymbol{x}')$ is a 0-1 diagonal matrix. We define the following events:

- $\mathcal{A}^h(\boldsymbol{x}, \boldsymbol{x}', \epsilon_1) := \{|\boldsymbol{g}^{(h)}(x^{(0)})^\top \boldsymbol{g}^{(h)}(\boldsymbol{x}) - \boldsymbol{\Sigma}^{(h)}(\boldsymbol{x}^{(0)}, \boldsymbol{x})| \leq \epsilon_1\}, \forall 0 \leq h \leq L$

- $\overline{\mathcal{A}}^h(\boldsymbol{x}, \boldsymbol{x}', \epsilon_1) = \mathcal{A}^h(\boldsymbol{x}, \boldsymbol{x}, \epsilon_1) \cap \mathcal{A}^h(\boldsymbol{x}, \boldsymbol{x}', \epsilon_1) \cap \mathcal{A}^h(\boldsymbol{x}', \boldsymbol{x}', \epsilon_1);$

- $\overline{\mathcal{A}}(\boldsymbol{x}, \boldsymbol{x}', \epsilon_1) = \bigcup_{h=0}^L \overline{\mathcal{A}}^h(\epsilon_1).$

- $\mathcal{B}^h(\boldsymbol{x}, \boldsymbol{x}', \epsilon_2) = \left\{ \left| \langle \mathbf{b}^{(h)}(\boldsymbol{x}), \mathbf{b}^{(h)}(\boldsymbol{x}') \rangle - \prod_{h=h}^L \dot{\Sigma}^{(h)}(\boldsymbol{x}, \boldsymbol{x}') \right| < \epsilon_2 \right\};$

- $\overline{\mathcal{B}}^h(\boldsymbol{x}, \boldsymbol{x}', \epsilon_2) = \mathcal{B}^h(\boldsymbol{x}, \boldsymbol{x}, \epsilon_2) \cap \mathcal{B}^h(\boldsymbol{x}, \boldsymbol{x}', \epsilon_2) \cap \mathcal{B}^h(\boldsymbol{x}', \boldsymbol{x}', \epsilon_2);$

- $\overline{\mathcal{B}}(\boldsymbol{x}, \boldsymbol{x}', \epsilon_2) = \bigcup_{h=1}^{L+1} \overline{\mathcal{B}}^h(\epsilon_2);$

- $\overline{\mathcal{C}}(\boldsymbol{x}, \boldsymbol{x}', \epsilon_3) = \{|f(\boldsymbol{\theta}, \boldsymbol{x})| \leq \epsilon_3, |f(\boldsymbol{\theta}, \boldsymbol{x}')| \leq \epsilon_3\};$

- $\mathcal{D}^h(\boldsymbol{x}, \boldsymbol{x}', \epsilon_4) = \left\{ |2\frac{\mathrm{tr}(\boldsymbol{D}(\boldsymbol{x},\boldsymbol{x}'))}{d_h} - \dot{\Sigma}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')| < \epsilon_4 \right\};$

- $\overline{\mathcal{D}}^h(\boldsymbol{x}, \boldsymbol{x}', \epsilon_4) = \mathcal{D}^h(\boldsymbol{x}, \boldsymbol{x}, \epsilon_4) \cap \mathcal{D}^h(\boldsymbol{x}, \boldsymbol{x}', \epsilon_4) \cap \mathcal{D}^h(\boldsymbol{x}', \boldsymbol{x}', \epsilon_1);$

- $\overline{\mathcal{D}}(\boldsymbol{x}, \boldsymbol{x}', \epsilon_4) = \bigcup_{h=1}^{L+1} \overline{\mathcal{D}}^h(\epsilon_4).$

For simplicity, we will omit $\boldsymbol{x}, \boldsymbol{x}'$ when there's no ambiguity. For events $\mathcal{A}, \mathcal{B}$, we define the event $\mathcal{A} \Rightarrow \mathcal{B}$ as $\neg \mathcal{A} \wedge \mathcal{B}$.

Lemma B.2. $\mathbb{P}[\mathcal{A} \Rightarrow \mathcal{B}] \geq \mathbb{P}[\mathcal{B} \mid \mathcal{A}].$

Proof. $\mathbb{P}[\mathcal{A} \Rightarrow \mathcal{B}] = \mathbb{P}[\neg \mathcal{A} \wedge \mathcal{B}] = 1 - \mathbb{P}[\mathcal{A} \vee \neg \mathcal{B}] = 1 - \mathbb{P}[\neg \mathcal{B} \mid \mathcal{A}]\mathbb{P}[\mathcal{A}] \geq 1 - \mathbb{P}[\neg \mathcal{B} \mid \mathcal{A}] = \mathbb{P}[\mathcal{B} \mid \mathcal{A}].$ $\square$

For matrix $\boldsymbol{A}$, define the projection matrix for the column space of $\boldsymbol{A}$, $\boldsymbol{\Pi_A} := \boldsymbol{A}\boldsymbol{A}^\dagger$ and the orthogonal projection matrix $\boldsymbol{\Pi}_{\boldsymbol{A}}^\perp = I - \boldsymbol{A}\boldsymbol{A}^\dagger$. For two random variables X and Y, $X \overset{\mathrm{d}}{=}_{\mathcal{A}} Y$ means X is equal to Y in distribution conditioned on the σ-algebra generated by $\mathcal{A}$.

Lemma B.3. *Let $\boldsymbol{w} \sim \mathcal{N}(0, \boldsymbol{I}_d)$, $\boldsymbol{G} \in \mathbb{R}^{d \times k}$ be some fixed matrix, and random vector $\boldsymbol{F} = \boldsymbol{w}^\top \boldsymbol{G}$, then conditioned on the value of $\boldsymbol{G}$, $\boldsymbol{w}$ remains gaussian in the null space of the row space of $\boldsymbol{G}$. Mathematically, it means*

$$\Pi_{\boldsymbol{G}}^\perp \boldsymbol{w} \overset{d}{=\!=}_{\boldsymbol{F} = \boldsymbol{w}^\top \boldsymbol{G}} \Pi_{\boldsymbol{G}}^\perp \widetilde{\boldsymbol{w}},$$

where $\widetilde{\boldsymbol{w}} \sim \mathcal{N}(0, \boldsymbol{I}_d)$ is a fresh i.i.d. copy of $\boldsymbol{w}$.

Proof. This lemma is straightforward when $\Pi_{\boldsymbol{G}}^\perp$ is a diagonal matrix.

In general, let $\boldsymbol{G} = \boldsymbol{U}\boldsymbol{G}'$, where $\boldsymbol{U} \in \mathbb{R}^{d \times d}$ is orthogonal and $\Pi_{G'}^\perp$ is diagonal. Now we have

$$\Pi_{\boldsymbol{G}}^\perp \boldsymbol{w} = \boldsymbol{U}\Pi_{\boldsymbol{G}'}^\perp \boldsymbol{U}^\top \boldsymbol{w} \overset{\mathrm{d}}{=\!=}_{\boldsymbol{F} = (\boldsymbol{U}^\top \boldsymbol{w})^\top \boldsymbol{G}'} \boldsymbol{U}\Pi_{\boldsymbol{G}'}^\perp \boldsymbol{U}^\top \widetilde{\boldsymbol{w}}, = \Pi_{\boldsymbol{G}}^\perp \widetilde{\boldsymbol{w}}$$

where we used the fact that if $\boldsymbol{w} \sim \mathcal{N}(0, \boldsymbol{I}_d)$, then for any orthogonal $\boldsymbol{U}$, $\boldsymbol{U}\boldsymbol{w} \sim \mathcal{N}(0, \boldsymbol{I}_d)$ twice. $\square$

B.2 Proof Sketch

Theorem 3.1 (Convergence to the NTK at initializatoin). *Fix $\epsilon > 0$ and $\delta \in (0,1)$. Suppose $\sigma(z) = \max(0, z)$ $(z \in \mathbb{R})$, $\min_{h \in [L]} d_h \geq \mathrm{poly}(L, 1/\epsilon) \cdot \log(L/\delta)$, and $[\boldsymbol{W}^{(h)}]_{i,j} \overset{i.i.d.}{\sim} \mathcal{N}(0, 1)$, $\forall h \in [L+1], i \in [d_h], j \in [d_{h-1}]$. Then for any inputs $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^{d_0}$ such that $\|\boldsymbol{x}\| \leq 1, \|\boldsymbol{x}'\| \leq 1$, with probability at least $1 - \delta$ we have:*

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

Proof. Recall that $\Theta^{(L)}(\boldsymbol{x}, \boldsymbol{x}') = \sum_{h=1}^{L+1} \left(\Sigma^{(h-1)}(\boldsymbol{x}, \boldsymbol{x}') \cdot \prod_{h'=h}^{L+1} \dot{\Sigma}^{(h')}(\boldsymbol{x}, \boldsymbol{x}') \right)$, thus it suffices to show that w.p. $1 - \epsilon$, for every $0 \leq h \leq L$, it holds that

$$\left| \left\langle \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{W}^{(h)}}, \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \boldsymbol{W}^{(h)}} \right\rangle - \Sigma^{(h-1)}(\boldsymbol{x}, \boldsymbol{x}') \cdot \prod_{h'=h}^{L+1} \dot{\Sigma}^{(h')}(\boldsymbol{x}, \boldsymbol{x}') \right| \leq \frac{\epsilon}{L+1},$$

which is a direct consequence of Theorem B.2 $\square$

Theorem B.1 (Corollary 16 in [Daniely et al., 2016]). *Let $\sigma(z) = \max(0, z), z \in \mathbb{R}$ and $[\boldsymbol{W}^{(h)}]_{ij} \overset{i.i.d.}{\sim} \mathcal{N}(0, 1)$, $\forall h \in [L], i \in [d^{h+1}], j \in [d^h]$, there exist constants c_1, c_2, such that if $c_1 \frac{L^2 \log\left(\frac{8L}{\delta}\right)}{\epsilon^2} \leq \min_{1 \leq h \leq L} d_h$ and $\epsilon \leq \min(c_2, \frac{1}{L})$, then for any fixed $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^{d_0}, \|\boldsymbol{x}\|, \|\boldsymbol{x}'\| \leq 1$, we have w.p. $\geq 1 - \delta$, $\forall 0 \leq h \leq L, \forall (\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \in \{(\boldsymbol{x}, \boldsymbol{x}), (\boldsymbol{x}, \boldsymbol{x}'), (\boldsymbol{x}', \boldsymbol{x}')\}$,*

$$\left| \boldsymbol{g}^{(h)}(\boldsymbol{x}^{(2)})^\top \boldsymbol{g}^{(h)}(\boldsymbol{x}^{(1)}) - \boldsymbol{\Sigma}^{(h)}(\boldsymbol{x}^{(2)}, \boldsymbol{x}^{(1)}) \right| \leq \epsilon.$$

In other words, if $\min_{h \in [L]} d_h \geq c_1 \frac{L^2 \log\left(\frac{L}{\delta_1}\right)}{\epsilon_1^2}$, $\epsilon_1 \leq \min(c_2, \frac{1}{L})$, then for fixed $\boldsymbol{x}, \boldsymbol{x}'$,

$$\mathbb{P}\left[\overline{\mathcal{A}}(\epsilon_1) \right] \geq 1 - \delta_1.$$

Theorem B.2. *Let* $\sigma(z) = \max(0, z), z \in \mathbb{R}$, *if* $[\boldsymbol{W}^{(h)}]_{ij} \overset{i.i.d.}{\sim} N(0,1), \forall h \in [L+1], i \in [d^{h+1}], j \in [d^h]$, *there exist constants* c_1, c_2, *such that if* $\min_{h \in [L]} d_h \geq c_1 \frac{L^2 \log(\frac{L}{\delta})}{\epsilon^4}, \epsilon \leq \frac{c_2}{L}$, *then for any fixed* $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^{d_0}, \|\boldsymbol{x}\|, \|\boldsymbol{x}'\| \leq 1$, *we have w.p.* $1 - \delta, \forall 0 \leq h \leq L, \forall (\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \in \{(\boldsymbol{x}, \boldsymbol{x}), (\boldsymbol{x}, \boldsymbol{x}'), (\boldsymbol{x}', \boldsymbol{x}')\}$,

$$\left| \boldsymbol{g}^{(h)}(\boldsymbol{x}^{(2)})^\top \boldsymbol{g}^{(h)}(\boldsymbol{x}^{(1)}) - \boldsymbol{\Sigma}^{(h)}(\boldsymbol{x}^{(2)}, \boldsymbol{x}^{(1)}) \right| \leq \frac{\epsilon^2}{2},$$

and

$$\left| \left\langle \mathbf{b}^{(h)}(\boldsymbol{x}^{(1)}), \mathbf{b}^{(h)}(\boldsymbol{x}^{(2)}) \right\rangle - \prod_{h'=h}^{L} \dot{\Sigma}^{(h')}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \right| < 3L\epsilon.$$

In other words, if $\min_{h \in [L]} d_h \geq c_1 \frac{L^2 \log(\frac{L}{\delta_1})}{\epsilon_1^2}$, $\epsilon_1 \leq \frac{c_2}{L}$, *then for fixed* $\boldsymbol{x}, \boldsymbol{x}'$,

$$\mathbb{P}\left[\overline{\mathcal{A}}\left(\frac{\epsilon^2}{8}\right) \bigwedge \overline{\mathcal{B}}(3L\epsilon) \right] \geq 1 - \delta$$

Note that for $c_\sigma = 2$ for $\sigma(z) = \max(0, z)$, by definition of $\mathbf{b}^{(h)}$, we have

$$\left\langle \mathbf{b}^{(h)}(\boldsymbol{x}), \mathbf{b}^{(h)}(\boldsymbol{x}') \right\rangle = \frac{2}{d_h} \mathbf{b}^{(h+1)}(\boldsymbol{x})^\top \boldsymbol{W}^{(h+1)} \boldsymbol{D}^{(h)}(\boldsymbol{x}) \boldsymbol{D}^{(h)}(\boldsymbol{x}') \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}').$$

Intuitively, when d_h is large, we can replace $\boldsymbol{W}^{(h+1)}$ by a fresh i.i.d copy $\widetilde{\boldsymbol{W}}$ with a small difference by $\tilde{O}(\frac{1}{\sqrt{d_h}})$ as below. Similar techniques are used in [Yang, 2019].

$$
\begin{aligned}
\left\langle \mathbf{b}^{(h)}(\boldsymbol{x}), \mathbf{b}^{(h)}(\boldsymbol{x}') \right\rangle &= \frac{2}{d_h} \mathbf{b}^{(h+1)}(\boldsymbol{x})^\top \boldsymbol{W}^{(h+1)} \boldsymbol{D}^{(h)}(\boldsymbol{x}) \boldsymbol{D}^{(h)}(\boldsymbol{x}') \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}') \\
&\approx \frac{2}{d_h} \mathbf{b}^{(h+1)}(\boldsymbol{x})^\top \widetilde{\boldsymbol{W}} \boldsymbol{D}^{(h)}(\boldsymbol{x}) \boldsymbol{D}^{(h)}(\boldsymbol{x}') \widetilde{\boldsymbol{W}}^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}') \\
&\approx \mathrm{tr}\left(\frac{2}{d_h} \boldsymbol{D}^{(h)}(\boldsymbol{x}) \boldsymbol{D}^{(h)}(\boldsymbol{x}') \right) \mathbf{b}^{(h+1)}(\boldsymbol{x})^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}') \\
&\approx \dot{\Sigma}^{(h)}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \prod_{h'=h+1}^{L} \dot{\Sigma}^{(h')}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)})
\end{aligned}
\tag{24}
$$

The proof is based on a careful control of the following events.

Lemma B.4.

$$\mathbb{P}\left[\overline{\mathcal{A}}^L\left(\epsilon_1^2/2\right) \Longrightarrow \overline{\mathcal{C}}\left(2\sqrt{\log \frac{4}{\delta_3}}\right) \right] \geq 1 - \delta_3, \quad \forall \epsilon_1 \in [0, 1], \delta_3 \in (0, 1).$$

Lemma B.5.

$$\mathbb{P}\left[\overline{\mathcal{A}}^{h+1}\left(\epsilon_1^2/2\right) \Longrightarrow \overline{\mathcal{D}}^h\left(\epsilon_1 + \sqrt{\frac{2\log\frac{6}{\delta_4}}{d_h}}\right) \right] \geq 1 - \delta_4, \quad \forall \epsilon_1 \in [0, 1], \delta_4 \in (0, 1).$$

Lemma B.6.

$$\mathbb{P}\left[\overline{\mathcal{A}}\left(\epsilon_1^2/2\right) \Longrightarrow \overline{\mathcal{D}}\left(\epsilon_1 + \sqrt{\frac{2\log\frac{6L}{\delta_4}}{\min_h d_h}}\right)\right] \geq 1 - \delta_4, \quad \forall \epsilon_1 \in [0,1], \delta_4 \in (0,1).$$

Proof. Apply union bound on Lemma B.5. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Lemma B.7. *There exists constant $C, C' \in \mathbb{R}$, for any $\epsilon_2, \epsilon_3, \epsilon_4 \in [0,1]$, we have*

$$\mathbb{P}\left[\overline{\mathcal{A}}^L\left(\epsilon_1^2/2\right) \bigwedge \overline{\mathcal{B}}^{h+1}\left(\epsilon_2\right) \bigwedge \overline{\mathcal{C}}\left(\epsilon_3\right) \bigwedge \overline{\mathcal{D}}^h\left(\epsilon_4\right) \Longrightarrow \overline{\mathcal{B}}^h\left(\epsilon_2 + \frac{C'\epsilon_3}{\sqrt{d_h}} + 2\epsilon_4 + C\sqrt{\frac{\log\frac{1}{\delta_2}}{d_h}}\right)\right] \geq 1 - \delta_2$$

Proof of Theorem B.2. We will use induction on Lemma B.7 to prove Theorem B.2. In the statement of Theorem B.1, we set $\delta_1 = \frac{\delta}{4}$, $\epsilon_1 = \frac{\epsilon^2}{8}$, for some c_1, c_2, we have

$$\mathbb{P}\left[\overline{\mathcal{A}}^L\left(\epsilon^2/8\right)\right] \geq 1 - \delta/4 \tag{25}$$

In the statement of Lemma B.6, we set $\delta_4 = \frac{\delta_2}{4}$, and $\epsilon_1 = \frac{\epsilon}{2}$. Note that for c_1 large enough $\sqrt{\frac{2\log\frac{24L}{\delta}}{\min_h d_h}} \leq \frac{\epsilon}{2}$ and thus we have

$$\mathbb{P}\left[\overline{\mathcal{A}}\left(\epsilon^2/8\right) \Rightarrow \overline{\mathcal{D}}\left(\epsilon\right)\right] \geq \mathbb{P}\left[\overline{\mathcal{A}}\left(\epsilon^2/8\right) \Rightarrow \overline{\mathcal{D}}\left(\epsilon/2 + \sqrt{\frac{2\log\frac{24L}{\delta}}{\min_h d_h}}\right)\right] \geq 1 - \delta/4 \tag{26}$$

In the statement of Lemma B.4, we set $\delta_3 = \frac{\delta}{4}$, and $\epsilon_1 = \frac{\epsilon^2}{8}$, we have

$$\mathbb{P}\left[\overline{\mathcal{A}}^L\left(\epsilon^2/8\right) \Rightarrow \overline{\mathcal{C}}\left(2\sqrt{\log\frac{16}{\delta}}\right)\right] \geq 1 - \delta/4 \tag{27}$$

Using union bound on Equation (25),(26),(27), we have

$$\mathbb{P}\left[\overline{\mathcal{A}}^L\left(\epsilon^2/8\right) \bigwedge \overline{\mathcal{C}}\left(2\sqrt{\log\frac{16}{\delta}}\right) \bigwedge \overline{\mathcal{D}}\left(\epsilon\right)\right] \geq 1 - \frac{3\delta}{4} \tag{28}$$

Now we will begin the induction argument. First of all, note that $\mathbb{P}\left[\overline{\mathcal{B}}^{L+1}\left(0\right)\right] = 1$ by definition.

For $1 \leq h \leq L$ in the statement of Lemma B.7, we set $\epsilon_2 = 3(L+1-h)\epsilon$, $\epsilon_3 = 3\sqrt{\log\frac{16}{\delta}}$, $\epsilon_2 = \epsilon$, $\delta_4 = \frac{\delta}{4L}$. Note that for c_1 large enough, $C\sqrt{\frac{\log\frac{1}{\delta_2}}{d_h}} + C'\sqrt{\frac{\log\frac{L}{\delta_2}}{d_h}} < \epsilon$. Thus we have

$$\mathbb{P}\left[\overline{\mathcal{B}}^{h+1}\left((3L-3h)\epsilon\right) \bigwedge \overline{\mathcal{C}}\left(3\sqrt{\log\frac{16}{\delta_2}}\right) \bigwedge \overline{\mathcal{D}}^h\left(\epsilon\right) \Rightarrow \overline{\mathcal{B}}^h\left((3L+2-3h)\epsilon + C\sqrt{\frac{\log\frac{1}{\delta}}{d_h}} + 3C'\sqrt{\frac{\log\frac{16}{\delta}}{d_h}}\right)\right]$$

$$\geq \mathbb{P}\left[\overline{\mathcal{B}}^{h+1}\left((3L-3h)\epsilon\right) \bigwedge \overline{\mathcal{C}}\left(3\sqrt{\log\frac{16}{\delta_2}}\right) \bigwedge \overline{\mathcal{D}}^h\left(\epsilon\right) \Rightarrow \overline{\mathcal{B}}^h\left((3L+3-3h)\epsilon\right)\right]$$

$$\geq 1 - \frac{\delta}{4L} \tag{29}$$

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Using union bound again on Equation (28) and Equation (29) for every h in $\{1, 2, \ldots, L\}$, we have

$$\mathbb{P}\left[\overline{\mathcal{A}}^L\left(\epsilon^2/8\right) \bigwedge \overline{\mathcal{C}}\left(\epsilon\right) \bigwedge \overline{\mathcal{D}}\left(\epsilon\right) \bigwedge \overline{\mathcal{B}}\left(3L\epsilon\right)\right]$$

$$\geq \mathbb{P}\left[\overline{\mathcal{A}}^L\left(\epsilon^2/8\right) \bigwedge \overline{\mathcal{C}}\left(\epsilon\right) \bigwedge \overline{\mathcal{D}}\left(\epsilon\right) \bigwedge_{h=1}^{L} \overline{\mathcal{B}}\left(3(L+1-h)\epsilon\right)\right]$$

$$\geq \left(1 - \mathbb{P}\left[\overline{\mathcal{A}}^L\left(\epsilon^2/8\right) \bigwedge \overline{\mathcal{C}}\left(\epsilon\right) \bigwedge \overline{\mathcal{D}}\left(\epsilon\right)\right]\right) \tag{30}$$

$$+ \sum_{h=1}^{L}\left(1 - \mathbb{P}\left[\overline{\mathcal{B}}^{h+1}\left((3L-3h)\epsilon\right) \bigwedge \overline{\mathcal{C}}\left(\epsilon\right) \bigwedge \overline{\mathcal{D}}^h\left(\epsilon\right) \Rightarrow \overline{\mathcal{B}}^h\left((3L+3-3h)\epsilon\right)\right]\right)$$

$$\geq 1 - \delta$$

$\square$

B.3   Proofs of Lemma B.4

Lemma B.4.

$$\mathbb{P}\left[\overline{\mathcal{A}}^L\left(\epsilon_1^2/2\right) \Longrightarrow \overline{\mathcal{C}}\left(2\sqrt{\log\frac{4}{\delta_3}}\right)\right] \geq 1 - \delta_3, \quad \forall \epsilon_1 \in [0, 1], \delta_3 \in (0, 1).$$

Proof. For fixed $\boldsymbol{g}^{(L)}(\boldsymbol{x})$, $f(\boldsymbol{\theta}, \boldsymbol{x}) = \boldsymbol{W}^{(L+1)}\boldsymbol{g}^{(L)}(\boldsymbol{x}) \stackrel{\mathrm{d}}{=} N\left(0, \left\|\boldsymbol{g}^{(L)}(\boldsymbol{x})\right\|^2\right)$. Thus by subgaussian concentration[cite], we know w.p. $\geq 1-\delta$ over the randomness of $\boldsymbol{W}^{(L+1)}$, $|f(\boldsymbol{\theta}, \boldsymbol{x})| \leq \sqrt{2\log\frac{2}{\delta}}\left\|\boldsymbol{g}^{(L)}(\boldsymbol{x})\right\|$.

For $\epsilon_1 \leq 1$, we have $\epsilon_1^2/2 < 1$, which implies $\left\|\boldsymbol{g}^{(L)}(\boldsymbol{x})\right\|^2 \leq 1 + \frac{\epsilon_1^2}{2} \leq 2$, and thus taking union bound over $\boldsymbol{x}, \boldsymbol{x}'$, we have w.p. $\geq 1 - \delta$, $|f(\boldsymbol{\theta}, \boldsymbol{x})| \leq 2\sqrt{\log\frac{2}{\delta}}, |f(\boldsymbol{\theta}, \boldsymbol{x}')| \leq 2\sqrt{\log\frac{2}{\delta}}$.

$$\mathbb{P}\left[\overline{\mathcal{A}}^L\left(\epsilon_1^2/2\right) \Rightarrow \overline{\mathcal{C}}\left(2\sqrt{\log\frac{4}{\delta_3}}\right)\right] \geq \mathbb{P}\left[\overline{\mathcal{C}}\left(2\sqrt{\log\frac{4}{\delta_3}}\right) \mid \overline{\mathcal{A}}^L\left(\epsilon_1^2/2\right)\right] \geq 1 - \delta$$

$\square$

B.4   Proofs for Lemma B.5

Lemma B.5.

$$\mathbb{P}\left[\overline{\mathcal{A}}^{h+1}\left(\epsilon_1^2/2\right) \Longrightarrow \overline{\mathcal{D}}^h\left(\epsilon_1 + \sqrt{\frac{2\log\frac{6}{\delta_4}}{d_h}}\right)\right] \geq 1 - \delta_4, \quad \forall \epsilon_1 \in [0, 1], \delta_4 \in (0, 1).$$

Lemma B.8. *Define* $\boldsymbol{G}^{(h)}(\boldsymbol{x}, \boldsymbol{x}') = \begin{bmatrix} \boldsymbol{g}^{(h)}(\boldsymbol{x})^\top\boldsymbol{g}^{(h)}(\boldsymbol{x}) & \boldsymbol{g}^{(h)}(\boldsymbol{x})^\top\boldsymbol{g}^{(h)}(\boldsymbol{x}') \\ \boldsymbol{g}^{(h)}(\boldsymbol{x}')^\top\boldsymbol{g}^{(h)}(\boldsymbol{x}) & \boldsymbol{g}^{(h)}(\boldsymbol{x}')^\top\boldsymbol{g}^{(h)}(\boldsymbol{x}') \end{bmatrix}$, *we have for every* $1 \leq h \leq L$,

$$\left\|\boldsymbol{G}^{(h)}(\boldsymbol{x}, \boldsymbol{x}') - \boldsymbol{\Lambda}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right\|_\infty \leq \frac{\epsilon^2}{2} \Rightarrow \left|t_{\dot{\sigma}}\left(\boldsymbol{G}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right) - t_{\dot{\sigma}}\left(\boldsymbol{\Lambda}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right)\right| \leq \epsilon, \forall 0 \leq \epsilon \leq 1.$$

Proof. For simplicity, we denote $\boldsymbol{G}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')$, $\boldsymbol{\Lambda}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')$ by $\boldsymbol{G}, \boldsymbol{\Lambda}$ respectively.

Since $\dot{\sigma}(z) = \mathbf{1}[z \geq 0]$ is 0-homogeneous, we have

$$t_{\dot{\sigma}}(\boldsymbol{G}) = \hat{t}_{\dot{\sigma}}\left(\frac{G_{12}}{\sqrt{G_{11}G_{22}}}\right) = \frac{1}{2} + \arcsin\frac{G_{12}}{\sqrt{G_{11}G_{22}}}$$

$$t_{\dot{\sigma}}(\boldsymbol{\Lambda}) = \hat{t}_{\dot{\sigma}}\left(\frac{\Lambda_{12}}{\sqrt{\Lambda_{11}\Lambda_{22}}}\right) = \frac{1}{2} + \arcsin\frac{\Lambda_{12}}{\sqrt{\Lambda_{11}\Lambda_{22}}} = \frac{1}{2} + \arcsin\Lambda_{12}$$

It is easy to verify that $|\sqrt{G_{11}G_{22}} - 1| \leq \epsilon^2/2$, and thus

$$\left|\frac{G_{12}}{\sqrt{G_{11}G_{22}}} - \Lambda_{12}\right| \leq \left|\frac{G_{12}}{\sqrt{G_{11}G_{22}}} - \frac{\Lambda_{12}}{\sqrt{G_{11}G_{22}}}\right| + |\Lambda_{12}|\left|1 - \frac{1}{\sqrt{G_{11}G_{22}}}\right| \leq \frac{\epsilon^2/2}{1-\epsilon^2/2} + \frac{\epsilon^2/2}{1-\epsilon^2/2} \leq 2\epsilon^2.$$

Thus, by Lemma B.1

$$|t_{\dot{\sigma}}(\boldsymbol{G}) - t_{\dot{\sigma}}(\boldsymbol{\Lambda})| \leq \left|\frac{1}{2} + \arcsin\frac{G_{12}}{\sqrt{G_{11}G_{22}}} - \frac{1}{2} + \arcsin\Lambda_{12}\right| \leq \epsilon.$$

$\square$

Lemma B.9. *For any $0 \leq h \leq L-1$, any fixed $\{\boldsymbol{W}^{(i)}\}_{i=1}^h$, w.p. $1-\delta$ over the randomness of $\boldsymbol{W}^{(h+1)} \in \mathbb{R}^{d^{h+1} \times d^h}$, we have*

$$\left|2\frac{\operatorname{tr}(\boldsymbol{D})}{d_h} - \hat{t}_{\dot{\sigma}}\left(\boldsymbol{G}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right)\right| < \sqrt{\frac{2\log\frac{2}{\delta}}{d_h}}.$$

Proof. Notice that $\mathbb{E}\left[2\frac{\operatorname{tr}(\boldsymbol{D})}{d_h}\right] = \hat{t}_{\dot{\sigma}}\left(\boldsymbol{G}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right)$, the proof is completed by Chernoff Bound. $\square$

Proof of Lemma B.5. Note that $\dot{\Sigma}^{(h)}(\boldsymbol{x}, \boldsymbol{x}') = t_{\sigma'}\left(\boldsymbol{\Sigma}^{(h)}\big|_{\boldsymbol{x},\boldsymbol{x}'}\right) = \hat{t}_{\sigma'}\left(\boldsymbol{\Lambda}^{(h)}(\boldsymbol{x}, \boldsymbol{x}')\right)$.

Combining Lemma B.8 and Lemma B.9, we have for any $(\boldsymbol{x}, \boldsymbol{x}')$,

$$\mathbb{P}\left[\mathcal{D}^h\left(\boldsymbol{x}, \boldsymbol{x}', \epsilon_1 + \sqrt{\frac{2\log\frac{6}{\delta}}{d_h}}\right) \mid \mathcal{A}^{h+1}\left(\boldsymbol{x}, \boldsymbol{x}', \epsilon_1^2/2\right)\right] \geq 1 - \frac{\delta}{3}.$$

Taking union bound over $(\boldsymbol{x}, \boldsymbol{x}), (\boldsymbol{x}, \boldsymbol{x}'), (\boldsymbol{x}', \boldsymbol{x}')$ for the choice of $(\boldsymbol{x}, \boldsymbol{x}')$, we have

$$\mathbb{P}\left[\overline{\mathcal{A}}^{h+1}\left(\epsilon_1^2/2\right) \Rightarrow \overline{\mathcal{D}}^h\left(\epsilon_1 + \sqrt{\frac{2\log\frac{6}{\delta}}{d_h}}\right)\right] \geq \mathbb{P}\left[\overline{\mathcal{D}}^h\left(\epsilon_1 + \sqrt{\frac{2\log\frac{6}{\delta}}{d_h}}\right) \mid \overline{\mathcal{A}}^{h+1}\left(\epsilon_1^2/2\right)\right] \geq 1 - \delta$$

$\square$

B.5 Proofs of Lemma B.7

Lemma B.7. *There exists constant $C, C' \in \mathbb{R}$, for any $\epsilon_2, \epsilon_3, \epsilon_4 \in [0,1]$, we have*

$$\mathbb{P}\left[\overline{\mathcal{A}}^L\left(\epsilon_1^2/2\right) \bigwedge \overline{\mathcal{B}}^{h+1}(\epsilon_2) \bigwedge \overline{\mathcal{C}}(\epsilon_3) \bigwedge \overline{\mathcal{D}}^h(\epsilon_4) \Longrightarrow \overline{\mathcal{B}}^h\left(\epsilon_2 + \frac{C'\epsilon_3}{\sqrt{d_h}} + 2\epsilon_4 + C\sqrt{\frac{\log\frac{1}{\delta_2}}{d_h}}\right)\right] \geq 1 - \delta_2$$

The proof of Lemma B.7 is based on the following 3 claims, Claim B.1, B.2 and B.3.

Claim B.1. *If $\overline{\mathcal{A}}^L\left(\epsilon_1^2/2\right) \bigwedge \overline{\mathcal{B}}^{h+1}(\epsilon_2) \bigwedge \overline{\mathcal{C}}(\epsilon_3) \bigwedge \overline{\mathcal{D}}^h(\epsilon_4)$, then we have*

$$\left| \frac{2\text{tr}(\boldsymbol{D})}{d_h} \left\langle \mathbf{b}^{(h)}(\boldsymbol{x}^{(2)}), \mathbf{b}^{(h)}(\boldsymbol{x}^{(1)}) \right\rangle - \prod_{h'=h}^{L} \dot{\Sigma}^{(h')}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \right| \leq \epsilon_2 + 2\epsilon_4.$$

Proof.

$$\left| \frac{2\text{tr}(\boldsymbol{D})}{d_h} \left\langle \mathbf{b}^{(h)}(\boldsymbol{x}^{(2)}), \mathbf{b}^{(h)}(\boldsymbol{x}^{(1)}) \right\rangle - \prod_{h'=h}^{L} \dot{\Sigma}^{(h')}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \right|$$

$$\leq \left| \frac{2\text{tr}(\boldsymbol{D})}{d_h} - \dot{\Sigma}^{(h)}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \right| \cdot \left| \left\langle \mathbf{b}^{(h)}(\boldsymbol{x}^{(2)}), \mathbf{b}^{(h)}(\boldsymbol{x}^{(1)}) \right\rangle \right|$$

$$+ \left| \dot{\Sigma}^{(h)}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \right| \cdot \left| \left\langle \mathbf{b}^{(h)}(\boldsymbol{x}^{(2)}), \mathbf{b}^{(h)}(\boldsymbol{x}^{(1)}) \right\rangle - \prod_{h'=h+1}^{L} \dot{\Sigma}^{(h')}(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \right|$$

$$\leq 2\epsilon_4 + \epsilon_2$$

$\square$

For any fixed h, let $\boldsymbol{G} = [\boldsymbol{g}^{(h)}(\boldsymbol{x}) \; \boldsymbol{g}^{(h)}(\boldsymbol{x}')]$,

Claim B.2. *w.p. $\geq 1 - \frac{\delta_2}{2}$, if $\overline{\mathcal{A}}^L\left(\epsilon_1^2/2\right) \bigwedge \overline{\mathcal{B}}^{h+1}(\epsilon_2) \bigwedge \overline{\mathcal{C}}(\epsilon_3) \bigwedge \overline{\mathcal{D}}^h(\epsilon_4)$, then we have for any $(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \in \{(\boldsymbol{x}, \boldsymbol{x}), (\boldsymbol{x}, \boldsymbol{x}'), (\boldsymbol{x}', \boldsymbol{x}')\}$,*

$$\left| \frac{2}{d_h} \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^\top \boldsymbol{W}^{(h+1)} \Pi_{\boldsymbol{G}}^\perp \boldsymbol{D} \Pi_{\boldsymbol{G}}^\perp \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)}) - \frac{2\text{tr}(\boldsymbol{D})}{d_h} \left\langle \mathbf{b}^{(h)}(\boldsymbol{x}^{(2)}), \mathbf{b}^{(h)}(\boldsymbol{x}^{(1)}) \right\rangle \right|$$

$$\leq 16\sqrt{\frac{\log\frac{6}{\delta_2}}{d_h}}.$$

As a by-product, for any $\boldsymbol{x}^{(1)} \in \{\boldsymbol{x}, \boldsymbol{x}'\}$, we have

$$\sqrt{\frac{2}{d_h}} \left\| \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^\top \boldsymbol{W}^{(h+1)} \Pi_{\boldsymbol{G}}^\perp \boldsymbol{D} \right\| \leq 4\sqrt{\frac{\log\frac{6}{\delta_2}}{d_h}}.$$

Lemma B.10 (Gaussian chaos of order 2, Boucheron et al. [2013]). *Let $\boldsymbol{\xi} \sim N(0, \boldsymbol{I}_n)$ be an n-dimensional unit gaussian random vector, $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ be a symmetric matrix, then for any $t > 0$,*

$$\mathbb{P}\left[\left|\boldsymbol{\xi}^\top \boldsymbol{A} \boldsymbol{\xi} - \mathbb{E}\left[\boldsymbol{\xi}^\top \boldsymbol{A} \boldsymbol{\xi}\right]\right| > 2\|\boldsymbol{A}\|_F \sqrt{t} + 2\|\boldsymbol{A}\|_2 t\right] \leq 2\exp(-t).$$

Or,

$$\mathbb{P}\left[\left|\boldsymbol{\xi}^\top \boldsymbol{A} \boldsymbol{\xi} - \mathbb{E}\left[\boldsymbol{\xi}^\top \boldsymbol{A} \boldsymbol{\xi}\right]\right| > t\right] \leq 2\exp\left(-\frac{t^2}{4(\|\boldsymbol{A}\|_F^2 + \|\boldsymbol{A}\|_2 t)}\right).$$

Proof of B.2. It suffices to prove this claim conditioned on every possible realization of

$$\{\mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)}), \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)}), \boldsymbol{f}^{(h)}(\boldsymbol{x}^{(1)}), \boldsymbol{f}^{(h)}(\boldsymbol{x}^{(2)})\}.$$

Recall that $\boldsymbol{G} = \begin{bmatrix} \boldsymbol{g}^{(h)}(\boldsymbol{x}^{(1)}) & \boldsymbol{g}^{(h)}(\boldsymbol{x}^{(2)}) \end{bmatrix}$, we further define $\boldsymbol{F} = \begin{bmatrix} \boldsymbol{f}^{(h)}(\boldsymbol{x}^{(1)}) & \boldsymbol{f}^{(h)}(\boldsymbol{x}^{(2)}) \end{bmatrix}$. Applying Lemma B.3 on each row of $\boldsymbol{W}^{h+1}$, we have

$$\boldsymbol{W}^{(h+1)}\Pi_{\boldsymbol{G}}^{\perp} \overset{\mathrm{d}}{=\!\!=}_{\boldsymbol{F}=\boldsymbol{W}^{(h+1)}\boldsymbol{G}} \widetilde{\boldsymbol{W}}\Pi_{\boldsymbol{G}}^{\perp}, \tag{31}$$

where $\widetilde{\boldsymbol{W}}$ is an iid copy of $\boldsymbol{W}^{(h+1)}$.

Note that $[\mathbf{b}^{(h+1)}(\boldsymbol{x})^{\top}\widetilde{\boldsymbol{W}} \quad \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^{\top}\widetilde{\boldsymbol{W}}]^{\top} \in \mathbb{R}^{2d_h}$ follows a joint zero-mean gaussian distribution with covariance matrix $\boldsymbol{\Sigma} = \begin{bmatrix} b_{11}\boldsymbol{I}_n & b_{12}\boldsymbol{I}_n \\ b_{21}\boldsymbol{I}_n & b_{22}\boldsymbol{I}_n \end{bmatrix}$, where $b_{ij} = \mathbf{b}^{(h)}(\boldsymbol{x}^{(i)})^{\top}\mathbf{b}^{(h)}(\boldsymbol{x}^{(j)})$, for $i, j = 1, 2$. In other words, there exists $\boldsymbol{M} \in \mathbb{R}^{2d_h \times 2d_h}$, s.t. $\boldsymbol{M}\boldsymbol{M}^{\top} = \boldsymbol{\Sigma}$, and

$$[\mathbf{b}^{(h+1)}(\boldsymbol{x})^{\top}\widetilde{\boldsymbol{W}} \quad \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^{\top}\widetilde{\boldsymbol{W}}]^{\top} \overset{\mathrm{d}}{=\!\!=} M\boldsymbol{\xi},$$

where $\boldsymbol{\xi} \sim N(\mathbf{0}, \boldsymbol{I}_{2d_h})$.

Thus conditioned on $\{\mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)}), \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)}), \boldsymbol{g}^{(h)}(\boldsymbol{x}^{(1)}), \boldsymbol{g}^{(h)}(\boldsymbol{x}^{(2)})\}$, we have

$$\mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^{\top}\boldsymbol{W}^{(h+1)}\Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp}\left(\boldsymbol{W}^{(h+1)}\right)^{\top}\mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)})$$

$$\overset{\mathrm{d}}{=\!\!=} \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^{\top}\widetilde{\boldsymbol{W}}\Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp}\left(\widetilde{\boldsymbol{W}}\right)^{\top}\mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)})$$

$$\overset{\mathrm{d}}{=\!\!=} \left(\begin{bmatrix} \boldsymbol{I}_{d_h} & \mathbf{0} \end{bmatrix}M\boldsymbol{\xi}\right)^{\top}\Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp}\left(\begin{bmatrix} \mathbf{0} & \boldsymbol{I}_{d_h} \end{bmatrix}M\boldsymbol{\xi}\right)$$

$$\overset{\mathrm{d}}{=\!\!=} \frac{1}{2}\boldsymbol{\xi}^{\top}M^{\top}\begin{bmatrix} \mathbf{0} & \Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp} \\ \Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp} & \mathbf{0} \end{bmatrix}M\boldsymbol{\xi}.$$

Now we are ready to prove Claim B.1 by applying Lemma B.10. Let $\boldsymbol{A} = \frac{1}{2}M^{\top}\begin{bmatrix} \mathbf{0} & \Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp} \\ \Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp} & \mathbf{0} \end{bmatrix}M$, we have

$$\mathbb{E}\left[\boldsymbol{\xi}^{\top}\boldsymbol{A}\boldsymbol{\xi}\right] = \mathrm{tr}\left(\boldsymbol{A}\right) = \frac{1}{2}\mathrm{tr}\left(\begin{bmatrix} \mathbf{0} & \Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp} \\ \Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp} & \mathbf{0} \end{bmatrix}\boldsymbol{\Sigma}\right) = b_{12}\mathrm{tr}\left(\Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{I}_n\right) = b_{12}\mathrm{tr}\left(\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp}\right).$$

Note that by definition $\Pi_{\boldsymbol{G}}^{\perp} = \boldsymbol{I}_{d_h} - \Pi_{\boldsymbol{G}}$, and $\mathrm{rank}(\Pi_{\boldsymbol{G}}) \le 2$, we have

$$\mathrm{tr}\left(\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp}\right) = \mathrm{tr}\left(\boldsymbol{D}(\boldsymbol{I} - \Pi_{\boldsymbol{G}})\right) = \mathrm{tr}\left(D\right) - \mathrm{tr}\left(\boldsymbol{D}\Pi_{\boldsymbol{G}}\right) = \mathrm{tr}\left(D\right) - \mathrm{tr}\left(\Pi_{\boldsymbol{G}}\boldsymbol{D}\Pi_{\boldsymbol{G}}\right).$$

Since $\mathbf{0} \preceq \boldsymbol{D} \preceq \boldsymbol{I}_{d_h}$, we have $0 \le \mathrm{tr}\left(\Pi_{\boldsymbol{G}}\boldsymbol{D}\Pi_{\boldsymbol{G}}\right) \le 2$, and thus $b_{12}(\mathrm{tr}\left(\boldsymbol{D}\right) - 2) \le \mathbb{E}\left[\boldsymbol{\xi}^{\top}\boldsymbol{A}\boldsymbol{\xi}\right] \le b_{12}\mathrm{tr}\left(\boldsymbol{D}\right)$. For the upper bound of spectrum, note that $\|\boldsymbol{M}\|_2^2 = \|\boldsymbol{\Sigma}\|_2 = \left\|\begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}\right\|_2 \le b_{11} + b_{12}$, and $\mathbf{0} \preceq \Pi_{\boldsymbol{G}}^{\perp}, \boldsymbol{D} \preceq \boldsymbol{I}_{d_h}$, we have

$$\|\boldsymbol{A}\|_2 \le \frac{1}{2}\|\boldsymbol{M}\|_2^2\left\|\Pi_{\boldsymbol{G}}^{\perp}\boldsymbol{D}\Pi_{\boldsymbol{G}}^{\perp}\right\|_2 \le \frac{1}{2}\|\boldsymbol{M}\|_2^2\left\|\Pi_{\boldsymbol{G}}^{\perp}\right\|_2\|\boldsymbol{D}\|_2\left\|\Pi_{\boldsymbol{G}}^{\perp}\right\|_2 \le \frac{b_{11} + b_{12}}{2} \le \sqrt{2},$$

and

$$\|\boldsymbol{A}\|_F \le \sqrt{2d_h}\|\boldsymbol{A}\|_2 = \frac{\sqrt{2d_h}(b_{11} + b_{22})}{2} \le 2\sqrt{d_h}.$$

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Thus by Lemma B.10 with $t = \log \frac{6}{\delta_2}$ we have w.p. $1 - \frac{\delta_2}{6}$,

$$\frac{1}{d_h} \left| \boldsymbol{\xi}^\top \boldsymbol{A} \boldsymbol{\xi} - \mathbb{E}\left[\boldsymbol{\xi}^\top \boldsymbol{A} \boldsymbol{\xi}\right] \right| \le \frac{1}{d_h} \left(2 \|\boldsymbol{A}\|_F \sqrt{t} + 2 \|\boldsymbol{A}\|_2 t \right) = 4\sqrt{\frac{\log \frac{6}{\delta_2}}{d_h}} + 2\sqrt{2}\frac{\log \frac{6}{\delta_2}}{d_h}..$$

Thus we have

$$\left| \frac{2}{d_h} \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^\top \boldsymbol{W}^{(h+1)} \Pi_{\boldsymbol{G}}^{\perp} \boldsymbol{D} \Pi_{\boldsymbol{G}}^{\perp} \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)}) - \frac{2\operatorname{tr}(\boldsymbol{D})}{d_h} \left\langle \mathbf{b}^{(h)}(\boldsymbol{x}^{(2)}), \mathbf{b}^{(h)}(\boldsymbol{x}^{(1)}) \right\rangle \right|$$

$$\le \frac{2}{d_h} \left| \boldsymbol{\xi}^\top \boldsymbol{A} \boldsymbol{\xi} - \mathbb{E}\left[\boldsymbol{\xi}^\top \boldsymbol{A} \boldsymbol{\xi}\right] \right| + \left| 2\mathbb{E}\left[\boldsymbol{\xi}^\top \boldsymbol{A} \boldsymbol{\xi}\right] - \frac{2\operatorname{tr}(\boldsymbol{D})}{d_h} \left\langle \mathbf{b}^{(h)}(\boldsymbol{x}^{(2)}), \mathbf{b}^{(h)}(\boldsymbol{x}^{(1)}) \right\rangle \right|$$

$$\le 8\sqrt{\frac{\log \frac{6}{\delta_2}}{d_h}} + 4\sqrt{2}\frac{\log \frac{6}{\delta_2}}{d_h} + \frac{4b_{12}}{d_h} \le 14\sqrt{\frac{\log \frac{6}{\delta_2}}{d_h}} + \frac{4(1+\epsilon_2)}{d_h} \quad (2\sqrt{2} \le 3 \wedge \log \frac{6}{\delta_2} \le d_h)$$

$$\le 16\sqrt{\frac{\log \frac{6}{\delta_2}}{d_h}} \quad (\epsilon_2 \le 1 \wedge \sqrt{d_h \log 6} \ge 4).$$

The main part of the claim is completed by taking union bound over $(\boldsymbol{x}, \boldsymbol{x}), (\boldsymbol{x}, \boldsymbol{x}'), (\boldsymbol{x}', \boldsymbol{x}')$. For the by-product, let $\boldsymbol{x}^{(2)} = \boldsymbol{x}^{(1)}$, and we have

$$\sqrt{\frac{2}{d_h}} \left\| \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^\top \boldsymbol{W}^{(h+1)} \Pi_{\boldsymbol{G}}^{\perp} \boldsymbol{D} \right\|$$

$$\le \sqrt{\left| \frac{2}{d_h} \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^\top \boldsymbol{W}^{(h+1)} \Pi_{\boldsymbol{G}}^{\perp} \boldsymbol{D} \Pi_{\boldsymbol{G}}^{\perp} \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)}) \right|}$$

$$\le \sqrt{\frac{2\operatorname{tr}(\boldsymbol{D})}{d_h} \left\langle \mathbf{b}^{(h)}(\boldsymbol{x}^{(2)}), \mathbf{b}^{(h)}(\boldsymbol{x}^{(1)}) \right\rangle + \left(16\sqrt{\frac{\log \frac{6}{\delta_2}}{d_h}}\right)^2}$$

$$\le \sqrt{4 + \left(16\sqrt{\frac{\log \frac{6}{\delta_2}}{d_h}}\right)^2}$$

$$\le 2 + 4\sqrt{\frac{\log \frac{6}{\delta_2}}{d_h}} \le 6 \quad (\log \frac{6}{\delta_2} \le d_h)$$

Claim B.3. *w.p.* $\ge 1 - \frac{\delta_2}{2}$, *if* $\overline{\mathcal{A}}^L\left(\epsilon_1^2/2\right) \bigwedge \overline{\mathcal{B}}^{h+1}\left(\epsilon_2\right) \bigwedge \overline{\mathcal{C}}\left(\epsilon_3\right) \bigwedge \overline{\mathcal{D}}^h\left(\epsilon_4\right)$, *then*

$$\left\| \Pi_{\boldsymbol{G}} \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}) \right\| \le 2\sqrt{\log \frac{8}{\delta_2}} + \sqrt{2}\epsilon_3, \left\| \Pi_{\boldsymbol{G}} \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}') \right\| \le 2\sqrt{\log \frac{8}{\delta_2}} + \sqrt{2}\epsilon_3.$$

Proof. It suffices to prove the claim for $\boldsymbol{x}$. We will denote $\boldsymbol{x}$ by $\boldsymbol{x}$, $\boldsymbol{g}^{(h)}(\boldsymbol{x})$ by $\boldsymbol{g}^{(h)}$ and $\mathbf{b}^{(h+1)}(\boldsymbol{x})$ by $\mathbf{b}^{(h+1)}$. We also define $\Pi_{\boldsymbol{g}}$ as $\boldsymbol{g}\boldsymbol{g}^\top$, and $\Pi_{\boldsymbol{G}/\boldsymbol{g}} = \Pi_{\boldsymbol{G}} - \Pi_{\boldsymbol{g}}$. Clearly, $\Pi_{\boldsymbol{G}/\boldsymbol{g}}$ is still a projection matrix of rank 0 or 1.

Since $\left\| \Pi_{\boldsymbol{G}} \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}) \right\| \le \left\| \Pi_{\boldsymbol{g}} \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}^{(h+1)} \right\| + \left\| \Pi_{\boldsymbol{G}/\boldsymbol{g}} \left(\boldsymbol{W}^{(h+1)}\right)^\top \mathbf{b}^{(h+1)} \right\|$, it suffices to bound these two terms separately.

Recall $\mathbf{b}^{(h+1)}$ is defined as the gradient of $f(\boldsymbol{\theta}, \boldsymbol{x})$ with respect to the pre-activation of layer $h+1$, $\boldsymbol{f}^{h+1}$, thus if we view g as a function $\boldsymbol{g}^{(h)}, \boldsymbol{W}^{(h+1)}, \ldots, \boldsymbol{W}^{(L+1)}$, by the rule of back propagation, we have

$$\frac{\partial g(\boldsymbol{g}^{(h)}, \boldsymbol{W}^{(h+1)}, \ldots, \boldsymbol{W}^{(L+1)})}{\partial \boldsymbol{g}^{(h)}} = (\mathbf{b}^{(h+1)})^\top \boldsymbol{W}^{(h+1)}.$$

Note that relu is 1-homogeneous, namely $\forall \lambda \in \mathbb{R}, \sigma(\lambda z) = \lambda \sigma(z)$, the whole network is also 1-homogeneous in $\boldsymbol{g}^{(h)}$. In other words, we have

$$
\begin{aligned}
&f(\boldsymbol{g}^{(h)}, \boldsymbol{W}^{(h+1)}, \ldots, \boldsymbol{W}^{(L+1)}) \\
&= \left. \frac{\partial f(\lambda \boldsymbol{g}^{(h)}, \boldsymbol{W}^{(h+1)}, \ldots, \boldsymbol{W}^{(L+1)})}{\partial \lambda} \right|_{\lambda=1} \\
&= \left\langle \left. \frac{\partial f(\lambda \boldsymbol{g}^{(h)}, \boldsymbol{W}^{(h+1)}, \ldots, \boldsymbol{W}^{(L+1)})}{\partial \lambda \boldsymbol{g}^{(h)}} \right|_{\lambda=1}, \left. \frac{\partial \lambda \boldsymbol{g}^{(h)}}{\partial \lambda} \right|_{\lambda=1} \right\rangle \\
&= \left\langle \frac{\partial g(\boldsymbol{g}^{(h)}, \boldsymbol{W}^{(h+1)}, \ldots, \boldsymbol{W}^{(L+1)})}{\partial \boldsymbol{g}^{(h)}}, \boldsymbol{g}^{(h)} \right\rangle \\
&= (\boldsymbol{g}^{(h)})^\top \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b}^{(h+1)}
\end{aligned}
$$

By definition of $\Pi_{\boldsymbol{g}}$, we have

$$\left\| \Pi_{\boldsymbol{g}} \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b} \right\| = \left\| \frac{\boldsymbol{g}^{(h)} (\boldsymbol{g}^{(h)})^\top}{\|\boldsymbol{g}^{(h)}\|^2} \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b}^{(h+1)}) \right\| = \left| \frac{(\boldsymbol{g}^{(h)})^\top}{\|\boldsymbol{g}^{(h)}\|} \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b}^{(h+1)}) \right| = \frac{|f(\boldsymbol{\theta}, \boldsymbol{x})|}{\|\boldsymbol{g}^{(h)}\|}.$$

Note that $\boldsymbol{g}^{(h)}(x^{(0)})^\top \boldsymbol{g}^{(h)}(\boldsymbol{x}) \geq 1 - \epsilon_1^2/2 \geq \frac{1}{2}$, we have

$$\left\| \Pi_{\boldsymbol{g}} \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b} \right\| = \frac{|f(\boldsymbol{\theta}, \boldsymbol{x})|}{\|\boldsymbol{g}^{(h)}\|} \leq \sqrt{2}\epsilon_3.$$

For the second term $\Pi_{\boldsymbol{G}/\boldsymbol{g}} \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b}^{(h+1)}$, note that conditioned on $\boldsymbol{g}^{(h)}$, $\boldsymbol{f}^h = \frac{1}{\sqrt{d_{h+1}}} \boldsymbol{W}^{(h+1)} \boldsymbol{g}^{(h)}$ and all $\{\boldsymbol{W}^{(h)}\}_{h'}^{L+1}$ (thus $\mathbf{b}^{(h+1)}$), by Lemma B.3, $\Pi_{\boldsymbol{G}/\boldsymbol{g}}(\boldsymbol{W}^{(h+1)}) \overset{d}{=} \Pi_{\boldsymbol{G}/\boldsymbol{g}} \widetilde{\boldsymbol{W}}$, where $\widetilde{\boldsymbol{W}}$ is an iid copy of $\boldsymbol{W}^{(h+1)}$. Thus if $\text{rank}(\Pi_{\boldsymbol{G}/\boldsymbol{g}}) = 1$, suppose $\Pi_{\boldsymbol{G}/\boldsymbol{g}} = \boldsymbol{u}\boldsymbol{u}^\top$ for some unit vector $\boldsymbol{u}$, we have

$$\left\| \Pi_{\boldsymbol{G}/\boldsymbol{g}} \left(\boldsymbol{W}^{(h+1)} \right)^\top \boldsymbol{b}^{(h+1)} \right\| = \left| \boldsymbol{u}^\top \left(\boldsymbol{W}^{(h+1)} \right)^\top \boldsymbol{b}^{(h+1)} \right| \overset{d}{=} \left| \boldsymbol{u}^\top \left(\widetilde{\boldsymbol{W}} \right)^\top \boldsymbol{b}^{(h+1)} \right| \overset{d}{=} |t|,$$

where $t \sim N(0, \|\boldsymbol{b}^{(h+1)}\|)$. Hence w.p. $\geq 1 - \delta_2/4$ over the randomness of $\boldsymbol{W}^{(L)}$, $\left\| \Pi_{\boldsymbol{G}/\boldsymbol{g}} \left(\boldsymbol{W}^{(h+1)} \right)^\top \boldsymbol{b}^{(h+1)} \right\| \leq \sqrt{2 \log \frac{8}{\delta_2}} \|\boldsymbol{b}^{(h+1)}\| \leq \sqrt{2 \log \frac{8}{\delta_2}} \leq 2 \sqrt{\log \frac{8}{\delta_2}}$ ($\epsilon_2 < 1$).

If $\text{rank}(\Pi_{\boldsymbol{G}/\boldsymbol{g}}) = 0$, then $\left\| \Pi_{\boldsymbol{G}/\boldsymbol{g}} \left(\boldsymbol{W}^{(h+1)} \right)^\top \boldsymbol{b}^{(h+1)} \right\| = 0 < 2\sqrt{\log \frac{8}{\delta_2}}$. Thus w.p. $\geq 1 - \frac{\delta_2}{4}$,

$$\left\| \Pi_{\boldsymbol{G}} \left(\boldsymbol{W}^{(h+1)} \right)^\top \boldsymbol{b}^{(h+1)}(\boldsymbol{x}) \right\| \leq \left\| \Pi_{\boldsymbol{g}} \left(\boldsymbol{W}^{(h+1)} \right)^\top \boldsymbol{b}^{(h+1)} \right\| + \left\| \Pi_{\boldsymbol{G}/\boldsymbol{g}} \left(\boldsymbol{W}^{(h+1)} \right)^\top \boldsymbol{b}^{(h+1)} \right\| \leq 2\sqrt{\log \frac{8}{\delta_2}} + \sqrt{2}\epsilon_3.$$

Thus by assumption $\log \frac{8}{\delta_2} \leq d_h$, we have $2\sqrt{\log \frac{8}{\delta_2}} + \sqrt{2}\epsilon_3 \leq 2\sqrt{d_h} + \sqrt{2} \leq 3\sqrt{2d_h}$. $\qquad \square$

Wrapping things up, by combining Claim B.2 and Claim B.3, we have w.p. $\geq 1 - \delta_2$, for any pair of $(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}) \in \{(\boldsymbol{x}, \boldsymbol{x}), (\boldsymbol{x}, \boldsymbol{x}'), (\boldsymbol{x}', \boldsymbol{x}'))\}$,

$$
\begin{aligned}
&\left| \frac{2}{d_h} \mathbf{b}^{(h+1)} (\boldsymbol{x}^{(1)})^\top \left(\boldsymbol{W}^{(h+1)} \right) \boldsymbol{D}^{(h)}(\boldsymbol{x}^{(1)}) \boldsymbol{D}^{(h)}(\boldsymbol{x}^{(2)}) \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)}) - \right. \\
&\left. \frac{2}{d_h} \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^\top \boldsymbol{W}^{(h+1)} \Pi_{\boldsymbol{G}}^\perp \boldsymbol{D} \Pi_{\boldsymbol{G}}^\perp \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)}) \right| \\
&\leq \left\| \frac{2}{d_h} \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^\top \boldsymbol{W}^{(h+1)} \Pi_{\boldsymbol{G}} \boldsymbol{D} \right\| \cdot \left\| \boldsymbol{D} \Pi_{\boldsymbol{G}}^\perp \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)}) \right\| \\
&+ \left\| \frac{2}{d_h} \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^\top \boldsymbol{W}^{(h+1)} \Pi_{\boldsymbol{G}}^\perp \boldsymbol{D} \right\| \cdot \left\| \boldsymbol{D} \Pi_{\boldsymbol{G}} \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)}) \right\| \\
&+ \left\| \frac{2}{d_h} \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(1)})^\top \boldsymbol{W}^{(h+1)} \Pi_{\boldsymbol{G}} \right\| \cdot \left\| \Pi_{\boldsymbol{G}} \left(\boldsymbol{W}^{(h+1)} \right)^\top \mathbf{b}^{(h+1)}(\boldsymbol{x}^{(2)}) \right\| \\
&\leq \left(12\sqrt{2} \sqrt{\frac{\ln \frac{8}{\delta_2}}{d_h}} + 12\epsilon_3 \right) + \left(12\sqrt{2} \sqrt{\frac{\ln \frac{8}{\delta_2}}{d_h}} + 12\epsilon_3 \right) + \left(12\sqrt{2} \sqrt{\frac{\ln \frac{8}{\delta_2}}{d_h}} + 12\epsilon_3 \right) \\
&= 36 \sqrt{\frac{2 \ln \frac{8}{\delta_2}}{d_h}} + 36\epsilon_3.
\end{aligned}
\tag{32}
$$

Using Equation (32) together with Claim B.1 and Claim B.2, we've finished the proof for Lemma B.7.

$\square$

C Proof of Theorem 3.2

In this section, we prove Theorem 3.2. At a high level, our proof first reduces the bounding the perturbation on the prediction to bounding perturbations on the kernel values between each pair of training points and between the testing point and each training point. We use the following notations. We let $\boldsymbol{X} \in \mathbb{R}^{n \times d}$ be the training data. We define $\ker_t(\boldsymbol{x}_{te}, \boldsymbol{X}) \in \mathbb{R}^n$ as

$$
[\ker_t (\boldsymbol{x}_{te}, \boldsymbol{X})]_i = \left\langle \frac{\partial f (\boldsymbol{\theta}(t), \boldsymbol{x}_{te})}{\partial \boldsymbol{\theta}}, \frac{\partial f (\boldsymbol{\theta}(t), \boldsymbol{x}_i)}{\partial \boldsymbol{\theta}} \right\rangle
$$

i.e., the kernel induced from the gradient of the prediction with respect to the parameters of the neural network at time t.

We also use the following notations for NTK. We let $\boldsymbol{H}^* \in \mathbb{R}^{n \times n}$ be the *fixed* kernel matrix defined in Equation (4). We let $\ker_{ntk} (\boldsymbol{x}_{te}, \boldsymbol{X}) \in \mathbb{R}^n$ be the kernel values between $\boldsymbol{x}_{te}$ and each training data. Note with this notation, we can write

$$
f_{ntk}(\boldsymbol{x}_{te}) = \ker_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{x})^\top (\boldsymbol{H}^*)^{-1} \boldsymbol{y}.
\tag{33}
$$

We prove a structural lemma to reduce the prediction perturbation bound to the kernel perturbation bound.

Lemma C.1 (Kernel Value Perturbation $\Rightarrow$ Prediction Perturbation). *Fix $\epsilon_{\boldsymbol{H}} \leq \frac{1}{2}\lambda_0$. Suppose $|f_{nn}(\boldsymbol{\theta}(0), \boldsymbol{x}_i)| \leq \epsilon_{init}$ for $i = 1, \ldots, n$ and $|f_{nn}(\boldsymbol{\theta}(0), \boldsymbol{x}_{te})| \leq \epsilon_{init}$ and $\|\boldsymbol{u}_{nn}(0) - \boldsymbol{y}\|_2 = O(\sqrt{n})$.*

Furthermore, if for all $t \geq 0$ $\|\ker_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{X}) - \ker_t(\boldsymbol{x}_{te}, \boldsymbol{X})\|_2 \leq \epsilon_{test}$ and $\|\boldsymbol{H}^* - \boldsymbol{H}(t)\|_2 \leq \epsilon_{\boldsymbol{H}}$, then we have

$$|f_{ntk}(\boldsymbol{x}_{te}) - f_{nn}(\boldsymbol{x}_{te})| \leq O\left(\epsilon_{init} + \frac{\sqrt{n}}{\lambda_0}\epsilon_{test} + \frac{\sqrt{n}}{\lambda_0^2}\log\left(\frac{n}{\epsilon_{\boldsymbol{H}}\lambda_0\kappa}\right)\epsilon_{\boldsymbol{H}}\right).$$

Proof of Lemma C.1. Our proof relies a careful analysis on the trajectories induced by gradient flows for optimizing the neural network and the NTK predictor.

Note while Equation (33) is a closed-form formula, we can rewrite it in an integral form using the following observations. For any $\boldsymbol{x} \in \mathbb{R}^d$, we let $\phi(\boldsymbol{x})$ be the feature map induced by NTK. Note the expression in Equation (33) can be rewritten as $f_{ntk}(\boldsymbol{x}_{te}) = \kappa\phi(\boldsymbol{x}_{te})^\top\boldsymbol{\beta}_{ntk}$ where $\boldsymbol{\beta}_{ntk}$ satisfies

$$\min_{\boldsymbol{\beta}} \|\boldsymbol{\beta}\|_2$$
$$\text{such that } \kappa\phi(\boldsymbol{x}_i)^\top\boldsymbol{\beta} = y_i \text{ for } i = 1, \ldots, n.$$

The solution to this program can written as applying gradient flow on

$$\min_{\boldsymbol{\beta}} \sum_{i=1}^n \frac{1}{2n}\left(\kappa\phi(\boldsymbol{x}_i)^\top\boldsymbol{\beta} - y_i\right)^2$$

with initialization $\boldsymbol{\beta}(0) = \boldsymbol{0}$. We use $\boldsymbol{\beta}(t)$ to denote this parameter at time t trained by gradient flow and $f_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{\beta}(t))$ be the predictor for $\boldsymbol{x}_{te}$ at time t. With these notations, we rewrite

$$f_{ntk}(\boldsymbol{x}_{te}) = \int_{t=0}^\infty \frac{df_{ntk}(\boldsymbol{\beta}(t), \boldsymbol{x}_{te})}{dt}dt$$

where we have used the fact that the initial prediction is 0. Now we take a closer look at the time derivative:

$$\frac{df_{ntk}(\boldsymbol{\beta}(t), \boldsymbol{x}_{te})}{dt} = \left\langle \frac{\partial f(\boldsymbol{\beta}(t), \boldsymbol{x}_{te})}{\partial\boldsymbol{\beta}(t)}, \frac{d\boldsymbol{\beta}(t)}{dt} \right\rangle$$

$$= \left\langle \frac{\partial f(\boldsymbol{\beta}(t), \boldsymbol{x}_{te})}{\partial\boldsymbol{\beta}(t)}, -\frac{\partial L(\boldsymbol{\beta}(t), \{\boldsymbol{x}_i\}_{i=1}^n)}{\partial\boldsymbol{\beta}(t)} \right\rangle$$

$$= -\frac{1}{n}\left\langle \frac{\partial f(\boldsymbol{\beta}(t), \boldsymbol{x}_{te})}{\partial\boldsymbol{\beta}(t)}, \sum_{i=1}^n (u_{ntk,i}(t) - y_i)\frac{\partial f(\boldsymbol{\beta}(t), \boldsymbol{x}_i)}{\boldsymbol{\beta}(t)} \right\rangle$$

$$= -\frac{1}{n}\left\langle \kappa\phi(\boldsymbol{x}_{te}), \sum_{i=1}^n (u_{ntk,i}(t) - y_i)\kappa\phi(\boldsymbol{x}_i) \right\rangle$$

$$= -\frac{\kappa^2}{n}\ker_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{X})^\top(\boldsymbol{u}_{ntk}(t) - \boldsymbol{y})$$

where $u_{ntk,i}(t) = f_{ntk}(\boldsymbol{\beta}(t), \boldsymbol{x}_i)$ and $\boldsymbol{u}_{ntk}(t) \in \mathbb{R}^n$ with $[\boldsymbol{u}_{ntk}(t)]_i = u_{ntk,i}(t)$. Similarly, for the NN predictor, we can obtain a time derivative of the same form.

$$\frac{df_{nn}(\boldsymbol{\theta}(t), \boldsymbol{x}_{te})}{dt} = \kappa\left\langle \frac{\partial f(\boldsymbol{\theta}(t), \boldsymbol{x}_{te})}{\partial\boldsymbol{\theta}(t)}, \frac{d\boldsymbol{\theta}(t)}{dt} \right\rangle$$

$$= \kappa\left\langle \frac{\partial f(\boldsymbol{\theta}(t), \boldsymbol{x}_{te})}{\partial\boldsymbol{\theta}(t)}, -\frac{\partial L(\boldsymbol{\theta}(t), \{\boldsymbol{x}_i\}_{i=1}^n)}{\partial\boldsymbol{\theta}(t)} \right\rangle$$

$$= -\frac{\kappa^2}{n} \left\langle \frac{\partial f(\boldsymbol{\theta}(t), \boldsymbol{x}_{te})}{\partial \boldsymbol{\theta}(t)}, \sum_{i=1}^{n} (u_{nn,i}(t) - y_i) \frac{\partial f(\boldsymbol{\theta}(t), \boldsymbol{x}_i)}{\boldsymbol{\theta}(t)} \right\rangle$$

$$= -\frac{\kappa^2}{n} \mathrm{ker}_t(\boldsymbol{x}_{te}, \boldsymbol{X})^\top (\boldsymbol{u}_{nn}(t) - \boldsymbol{y})$$

We thus we analyze the difference between the NN predictor and NTK predictor via this integral form

$$|f_{nn}(\boldsymbol{x}_{te}) - f_{ntk}(\boldsymbol{x}_{te})|$$

$$= \left| f_{nn}(\boldsymbol{\theta}(0), \boldsymbol{x}_{te}) + \int_{t=0}^{\infty} \left(\frac{df_{nn}(\boldsymbol{\theta}(t), \boldsymbol{x}_{te})}{dt} - \frac{df_{ntk}(\boldsymbol{\beta}(t), \boldsymbol{x}_{te})}{dt} \right) dt \right|$$

$$= \left| f_{nn}(\boldsymbol{\theta}(0), \boldsymbol{x}_{te}) \right| + \left| -\frac{\kappa^2}{n} \int_{t=0}^{\infty} \left(\mathrm{ker}_t(\boldsymbol{x}_{te}, \boldsymbol{X})^\top (\boldsymbol{u}_{nn}(t) - \boldsymbol{y}) - \mathrm{ker}_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{X})^\top (\boldsymbol{u}_{ntk}(t) - \boldsymbol{y}) \right) dt \right|$$

$$\leq \epsilon_{init} + \frac{\kappa^2}{n} \left| \int_{t=0}^{\infty} (\mathrm{ker}_t(\boldsymbol{x}_{te}, \boldsymbol{X}) - \mathrm{ker}_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{X}))^\top (\boldsymbol{u}_{nn}(t) - \boldsymbol{y}) dt \right|$$

$$+ \frac{\kappa^2}{n} \left| \int_{t=0}^{\infty} \mathrm{ker}_{ntk}(\boldsymbol{x}_t, \boldsymbol{X})^\top (\boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t)) dt \right|$$

$$\leq \epsilon_{init} + \kappa^2 \max_{0 \leq t \leq \infty} \|\mathrm{ker}_t(\boldsymbol{x}_{te}, \boldsymbol{X}) - \mathrm{ker}_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{X})\|_2 \int_{t=0}^{\infty} \|\boldsymbol{u}_{nn}(t) - \boldsymbol{y}\|_2 dt$$

$$+ \kappa^2 \max_{0 \leq t \leq \infty} \|\mathrm{ker}_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{X})\|_2 \int_{t=0}^{\infty} \|\boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t)\|_2 dt$$

$$\leq \epsilon_{init} + \kappa^2 \epsilon_{test} \int_{t=0}^{\infty} \|\boldsymbol{u}_{nn}(t) - \boldsymbol{y}\|_2 dt + \kappa^2 \max_{0 \leq t \leq \infty} \|\mathrm{ker}_{ntk}(\boldsymbol{x}_{te}, \boldsymbol{X})\|_2 \int_{t=0}^{\infty} \|\boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t)\|_2 dt$$

For the second term, recall $\|\boldsymbol{H}^* - \boldsymbol{H}(t)\|_2 \leq \epsilon_{\boldsymbol{H}}$ by our assumption so $\lambda_{\min}(\boldsymbol{H}(t)) \geq \frac{1}{2}\lambda_0$. Using this fact we know $\|\boldsymbol{u}_{nn}(t) - \boldsymbol{y}\|_2 \leq \exp(-\frac{\kappa^2}{2}\lambda_0 t) \|\boldsymbol{u}_{nn}(0) - \boldsymbol{y}\|_2$. Therefore, we can bound

$$\int_0^{\infty} \|\boldsymbol{u}_{nn}(t) - \boldsymbol{y}\|_2 dt = \int_{t=0}^{\infty} \exp(-\frac{\kappa^2}{2}\lambda_0 t) \|\boldsymbol{u}_{nn}(0) - \boldsymbol{y}\|_2 dt = O\left(\frac{\sqrt{n}}{\kappa^2 \lambda_0} \right).$$

To bound $\int_{t=0}^{\infty} \|\boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t)\|_2$, we observe that $\boldsymbol{u}_{nn}(t) \to \boldsymbol{y}$ and $\boldsymbol{u}_{ntk}(t) \to \boldsymbol{y}$ with linear convergence rate. Therefore, we can choose some $t_0 = \frac{C}{\lambda_0 \kappa^2} \log\left(\frac{n}{\epsilon_{\boldsymbol{H}} \lambda_0 \kappa} \right)$ so that

$$\int_{t_0}^{\infty} \|\boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t)\|_2 dt$$

$$\leq \int_{t_0}^{\infty} \|\boldsymbol{u}_{nn}(t) - \boldsymbol{y}\|_2 dt + \int_{t_0}^{\infty} \|\boldsymbol{u}_{ntk}(t) - \boldsymbol{y}\|_2 dt$$

$$\leq O\left(\frac{1}{\lambda_0 \kappa^2} \left(\|\boldsymbol{u}_{nn}(t_0) - \boldsymbol{y}\|_2 + \|\boldsymbol{u}_{ntk}(t_0) - \boldsymbol{y}\|_2 \right) \right)$$

$$\leq O\left(\frac{\sqrt{n}}{\lambda_0 \kappa} \exp\left(-\lambda_0 \kappa^2 t_0 \right) \right)$$

$$\leq O(\epsilon_{\boldsymbol{H}}).$$

Thus it suffices to bound

$$\int_{t=0}^{t_0} \left\| \boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t) \right\|_2 dt \le t_0 \max_{0 \le t \le t_0} \left\| \boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t) \right\|_2 .$$

First observe that

$$\begin{aligned} &\left\| \boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t) \right\|_2 \\ &\le \left\| \boldsymbol{u}_{nn}(0) \right\|_2 + \int_{\tau=0}^{t} \left\| \frac{d\left(\boldsymbol{u}_{nn}(\tau) - \boldsymbol{u}_{ntk}(\tau) \right)}{d\tau} \right\|_2 d\tau \\ &\le \epsilon_{init}\sqrt{n} + \int_{\tau=0}^{t} \left\| \frac{d\left(\boldsymbol{u}_{nn}(\tau) - \boldsymbol{u}_{ntk}(\tau) \right)}{d\tau} \right\|_2 d\tau. \end{aligned}$$

Note

$$\begin{aligned} &\frac{d\left(\boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t) \right)}{dt} \\ &= -\kappa^2 \boldsymbol{H}(t) \left(\boldsymbol{u}_{nn}(t) - \boldsymbol{y} \right) + \kappa^2 \boldsymbol{H}^* \left(\boldsymbol{u}_{ntk}(t) - \boldsymbol{y} \right) \\ &= -\kappa^2 \boldsymbol{H}^* \left(\boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t) \right) + \kappa^2 \left(\boldsymbol{H}^* - \boldsymbol{H}(t) \right) \left(\boldsymbol{u}_{nn}(t) - \boldsymbol{y} \right) \end{aligned}$$

Since $\boldsymbol{H}^*$ is positive semidefinite, $-\boldsymbol{H}^* \left(\tilde{\boldsymbol{u}}(t) - \boldsymbol{u}(t) \right)$ term only makes $\left\| \tilde{\boldsymbol{u}}(t) - \boldsymbol{u}(t) \right\|_2$ smaller. Therefore, we have

$$\begin{aligned} \left\| \boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t) \right\|_2 &\le \kappa^2 \int_{\tau=0}^{t} \left\| \boldsymbol{u}_{nn}(\tau) - \boldsymbol{y} \right\|_2 \left\| \boldsymbol{H}(t) - \boldsymbol{H}^* \right\|_2 \\ &\le t\kappa^2 \left\| \boldsymbol{u}_{nn}(0) - \boldsymbol{y} \right\|_2 \epsilon_{\boldsymbol{H}} \\ &\le O\left(t\kappa^2 \sqrt{n} \epsilon_{\boldsymbol{H}} \right). \end{aligned}$$

Therefore, we have

$$\int_{t=0}^{t_0} \left\| \boldsymbol{u}_{nn}(t) - \boldsymbol{u}_{ntk}(t) \right\|_2 dt \le O\left(t_0^2 \sqrt{n} \kappa^2 \epsilon_{\boldsymbol{H}} \right) = O\left(\frac{\sqrt{n}}{\lambda_0^2 \kappa^2} \log\left(\frac{n}{\epsilon_{\boldsymbol{H}} \lambda_0 \kappa} \right) \epsilon_{\boldsymbol{H}} \right).$$

Lastly, we put things together and get

$$\left| f_{ntk}(\boldsymbol{x}_{te}) - f_{nn}(\boldsymbol{x}_{te}) \right| \le O\left(\epsilon_{init} + \epsilon_{test} \frac{\sqrt{n}}{\lambda_0} + \frac{\sqrt{n}}{\lambda_0^2} \log\left(\frac{n}{\epsilon_{\boldsymbol{H}} \lambda_0 \kappa} \right) \epsilon_{\boldsymbol{H}} \right).$$

$\square$

By Lemma C.1, the problem now reduces to 1) choose κ small enough to make $\epsilon_{init} = O(\epsilon)$ and 2) show when the width is large enough then $\epsilon_{\boldsymbol{H}}$ and ϵ_{test} are both $O(\epsilon)$. For 1), based on Theorem B.1 and the union bound, we can just choose $\kappa = O\left(\frac{\epsilon}{\log(n/\delta)} \right)$ to make $\epsilon_{init} = O(\epsilon)$ with probability $1 - \delta$. For 2), we will use Theorem 3.1 and Theorem D.1 and then apply the union bound.

D   Proof of Convergence to NTK During Training

Theorem D.1 (Kernel Perturbation Bound During Training). *Fix $\omega \leq \text{poly}(1/L, 1/n, 1/\log(1/\delta), \lambda_0)$. Suppose we set $m \geq \text{poly}(1/\omega)$ and $\kappa \leq 1$. Then with probability at least $1 - \delta$ over random initialization, we have for all $t \geq 0$, for any $(\boldsymbol{x}, \boldsymbol{x}') \in \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n, \boldsymbol{x}_{te}\} \times \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n, \boldsymbol{x}_{te}\}$*

$$\left|\ker_t\left(\boldsymbol{x}, \boldsymbol{x}'\right) - \ker_0\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right| \leq \omega$$

Recall for any fixed $\boldsymbol{x}$ and $\boldsymbol{x}'$, Theorem 3.1 shows $|\ker_0(\boldsymbol{x}, \boldsymbol{x}') - \ker_{ntk}(\boldsymbol{x}, \boldsymbol{x}')| \leq \epsilon$ if m is large enough. The next lemma shows we can reduce the problem of bounding the perturbation on the kernel value to the perturbation on the gradient.

Lemma D.1 (Gradient Perturbation $\to$ Kernel Perturbation). *If $\left\|\frac{\partial f(\boldsymbol{\theta}(y), \boldsymbol{x})}{\partial \boldsymbol{\theta}} - \frac{\partial f(\boldsymbol{\theta}(0), \boldsymbol{x})}{\partial \boldsymbol{\theta}}\right\| \leq \epsilon$ and $\left\|\frac{\partial f(\boldsymbol{\theta}(t), \boldsymbol{x}')}{\partial \boldsymbol{\theta}} - \frac{\partial f(\boldsymbol{\theta}(0), \boldsymbol{x}')}{\partial \boldsymbol{\theta}}\right\| \leq \epsilon$, we have*

$$\left|\ker_t(\boldsymbol{x}, \boldsymbol{x}') - \ker_0(\boldsymbol{x}, \boldsymbol{x}')\right| \leq O\left(\epsilon\right)$$

Proof of Lemma D.1. By the proof of Theorem 3.1, we know $\left\|\frac{\partial f(\boldsymbol{\theta}(0), \boldsymbol{x})}{\partial \boldsymbol{\theta}}\right\|_2 = O\left(1\right)$. Then we can just use triangle inequality. $\square$

Now we proceed to analyze the perturbation on the gradient. Note we can focus on the perturbation on a single sample $\boldsymbol{x}$ because we can later take a union bound. Therefore, in the rest of this section, we drop the dependency on a specific sample. We use the following notations in this section. Recall $\boldsymbol{W}^{(1)}, \ldots, \boldsymbol{W}^{(L+1)} \sim \mathcal{N}\left(\boldsymbol{0}, \boldsymbol{I}\right)$ and we denote $\triangle \boldsymbol{W}^{(1)}, \ldots, \triangle \boldsymbol{W}^{(L+1)}$ the perturbation matrices. We let $\widetilde{\boldsymbol{W}}^{(h)} = \boldsymbol{W}^{(h)} + \triangle \boldsymbol{W}^{(h)}$. We let $\tilde{\boldsymbol{g}}^{(0)} = \boldsymbol{g}^{(0)} = \boldsymbol{x}$ and for $h = 1, \ldots, L$ we define

$$\boldsymbol{z}^{(h)} = \sqrt{\frac{2}{m}} \boldsymbol{W}^{(h)} \boldsymbol{g}^{(h-1)}, \quad \boldsymbol{g}^{(h)} = \sigma\left(\boldsymbol{z}^{(h)}\right),$$

$$\tilde{\boldsymbol{z}}^{(h)} = \sqrt{\frac{2}{m}} \widetilde{\boldsymbol{W}}^{(h)} \tilde{\boldsymbol{g}}^{(h-1)}, \quad \tilde{\boldsymbol{g}}^{(h)} = \sigma\left(\tilde{\boldsymbol{z}}^{(h)}\right).$$

For $h = 1, \ldots, L$, $i = 1, \ldots, m$, we denote

$$[\boldsymbol{D}^{(h)}]_{ii} = \mathbb{1}\left\{\left[\boldsymbol{W}^{(h)}\right]_{i,:} \boldsymbol{g}^{(h-1)} \geq 0\right\}$$

$$[\widetilde{\boldsymbol{D}}^{(h)}]_{ii} = \mathbb{1}\left\{\left[\widetilde{\boldsymbol{W}}^{(h)}\right]_{i,:} \tilde{\boldsymbol{g}}^{(h-1)} \geq 0\right\}.$$

Remark D.1. *Note $\boldsymbol{z}^{(h)} = \sqrt{\frac{2}{m}} \boldsymbol{f}^{(h)}$. Here we use $\boldsymbol{z}^{(h)}$ instead of $\boldsymbol{f}^{(h)}$ for the ease of presentation.*

For convenience, we also define

$$\triangle \boldsymbol{D}^{(h)} = \widetilde{\boldsymbol{D}}^{(h)} - \boldsymbol{D}^{(h)}.$$

Recall the gradient to $\boldsymbol{W}^{(h)}$ is:

$$\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{W}^{(h)}} = \boldsymbol{b}^{(h)} \left(\boldsymbol{g}^{(h-1)}\right)^{\top}$$

Similarly, we have

$$\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \widetilde{\boldsymbol{W}}^{(h)}} = \tilde{\boldsymbol{b}}^{(h)} \left(\tilde{\boldsymbol{g}}^{(h-1)} \right)^{\top}$$

where

$$\tilde{\boldsymbol{b}}^{(h)} = \begin{cases} 1 & \text{if } h = L+1 \\ \sqrt{\frac{2}{m}} \widetilde{\boldsymbol{D}}^{(h)} \left(\widetilde{\boldsymbol{W}}^{(h+1)} \right)^{\top} \tilde{\boldsymbol{b}}^{(h+1)} & \text{Otherwise} \end{cases}.$$

This gradient formula allows us to bound the perturbation on $\triangle \boldsymbol{g}^{(h)} \triangleq \tilde{\boldsymbol{g}}^{(h)} - \boldsymbol{g}^{(h)}$ and $\triangle \boldsymbol{b}^{(h)} \triangleq \tilde{\boldsymbol{b}}^{(h)} - \boldsymbol{b}^{(h)}$ separately. The following lemmas adapted from Allen-Zhu et al. [2018b] show with high probability over the initialization, bounding the perturbation on $\triangle \boldsymbol{g}^{(h)}$ and $\triangle \boldsymbol{b}^{(h)}$ can be reduced to bounding the perturbation on weight matrices.

Lemma D.2 (Adapted from Lemma 5.2 of Allen-Zhu et al. [2018b]). *Suppose*

$$\omega \le \text{poly} \left(1/n, \lambda_0, 1/L, 1/\log(m), \epsilon, 1/\log(1/\delta) \right).$$

Then with probability at least $1 - \delta$ over random initialization, if $\left\| \triangle \boldsymbol{W}^{(h)} \right\|_2 \le \sqrt{m} \omega$ for all $h = 1, \dots, L$, we have $\left\| \triangle \boldsymbol{g}^{(h)} \right\|_2 = O(\omega L^{5/2} \sqrt{\log m})$ for all $h = 1, \dots, L$.

Remark D.2. *While Allen-Zhu et al. [2018b] did not consider the perturbation on $\boldsymbol{W}^{(1)}$, by scrutinizing their proof, it is easy to see that the perturbation bounds still hold even if there is a small perturbation on $\boldsymbol{W}^{(1)}$.*

The next lemma bounds the backward vector, adapted from

Lemma D.3 (Adapted from Lemma 5.7 of Allen-Zhu et al. [2018b]). *Suppose*

$$\omega \le \text{poly} \left(1/n, \lambda_0, 1/L, 1/\log(m), \epsilon, 1/\log(1/\delta) \right).$$

Then with probability at least $1 - \delta$ over random initialization, if $\left\| \triangle \boldsymbol{W}^{(h)} \right\|_2 \le \sqrt{m} \omega$ for all $h = 1, \dots, L+1$, we have for all $h = 1, \dots, L+1$, $\left\| \tilde{\boldsymbol{b}}^{(h)} - \boldsymbol{b}^{(h)} \right\|_2 = O \left(\omega^{1/3} L^2 \sqrt{\log m} \right)$.

Remark D.3. *While Allen-Zhu et al. [2018b] did not consider the perturbation on $\boldsymbol{W}^{(L+1)}$, by scrutinizing their proof, it is easy to see that the perturbation bounds still hold even if there is a small perturbation on $\boldsymbol{W}^{(L+1)}$.*

Combing these two lemmas and the result for the initialization (Theorem 3.1), we have the following "gradient-Lipschitz" lemma.

Lemma D.4. *Suppose $\omega \le \text{poly} \left(1/n, \lambda_0, 1/L, 1/\log(m), \epsilon, 1/\log(1/\delta) \right)$. Then with probability at least $1 - \delta$ over random initialization, if $\left\| \triangle \boldsymbol{W}^{(h)} \right\|_2 \le \sqrt{m} \omega$ for all $h = 1, \dots, L+1$, we have for all $h = 1, \dots, L+1$:*

$$\left\| \tilde{\boldsymbol{b}}^{(h)} \left(\tilde{\boldsymbol{g}}^{(h-1)} \right)^{\top} - \boldsymbol{b}^{(h)} \left(\boldsymbol{g}^{(h-1)} \right)^{\top} \right\|_F = O \left(\omega^{1/3} L^{5/2} \sqrt{\log m} \right)$$

Proof of Lemma D.4. We use the triangle inequality to bound the perturbation

$$\left\| \tilde{\boldsymbol{b}}^{(h)} \left(\tilde{\boldsymbol{g}}^{(h-1)} \right)^{\top} - \boldsymbol{b}^{(h)} \left(\boldsymbol{g}^{(h-1)} \right)^{\top} \right\|_F$$

$$\leq \left\| \tilde{\boldsymbol{b}}^{(h)} \left(\tilde{\boldsymbol{g}}^{(h-1)} \right)^{\top} - \boldsymbol{b}^{(h)} \left(\tilde{\boldsymbol{g}}^{(h-1)} \right)^{\top} \right\|_F + \left\| \boldsymbol{b}^{(h)} \left(\tilde{\boldsymbol{g}}^{(h-1)} \right)^{\top} - \boldsymbol{b}^{(h)} \left(\boldsymbol{g}^{(h-1)} \right)^{\top} \right\|_F$$

$$\leq \left\| \triangle \boldsymbol{b}^{(h)} \left(\boldsymbol{g}^{(h-1)} + \triangle \boldsymbol{g}^{(h-1)} \right)^{\top} \right\|_F + \left\| \boldsymbol{b}^{(h)} \left(\triangle \boldsymbol{g}^{(h-1)} \right)^{\top} \right\|_F$$

$$= O \left(\omega^{1/3} L^{5/2} \sqrt{\log m} \right).$$

$\square$

The following lemma shows for given weight matrix, if we have linear convergence and other weight matrices are only perturbed by a little, then the given matrix is only perturbed by a little as well.

Lemma D.5. *Fix $h \in [L+1]$ and a sufficiently small $\omega \leq \text{poly}\left(1/n, \lambda_0, 1/L, 1/\log(m), \epsilon, 1/\log(1/\delta), \kappa\right)$. Suppose for all $t \geq 0$, $\|\boldsymbol{u}_{nn}(t) - \boldsymbol{y}\|_2 \leq \exp\left(-\frac{1}{2}\kappa^2\lambda_0 t\right) \|\boldsymbol{u}_{nn}(0) - \boldsymbol{y}\|_2$ and $\left\| \boldsymbol{W}^{(h')}(t) - \boldsymbol{W}^{(h')}(0) \right\|_F \leq \omega\sqrt{m}$ for $h' \neq h$. Then if $m \geq \text{poly}\left(1/\omega\right)$ we have with probability at least $1 - \delta$ over random initialization, for all $t \geq 0$*

$$\left\| \boldsymbol{W}^{(h)}(t) - \boldsymbol{W}^{(h)}(0) \right\|_F = O \left(\frac{\sqrt{n}}{\lambda_0} \right) \leq \omega\sqrt{m}.$$

Proof of Lemma D.5. We let $C, C_0, C_1, C_2, C_3 > 0$ be some absolute constants.

$$\left\| \boldsymbol{W}^{(h)}(t) - \boldsymbol{W}^{(h)}(0) \right\|_F$$

$$= \left\| \int_0^t \frac{d\boldsymbol{W}^{(h)}(\tau)}{d\tau} d\tau \right\|_F$$

$$= \left\| \int_0^t \frac{\partial L(\boldsymbol{\theta}(\tau))}{\partial \boldsymbol{W}^{(h)}(\tau)} d\tau \right\|_F$$

$$= \left\| \int_0^t \frac{1}{n} \sum_{i=1}^n (u_i(\tau) - y_i) \frac{\partial f_{nn}(\boldsymbol{\theta}(\tau), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} d\tau \right\|_F$$

$$\leq \frac{1}{n} \max_{0 \leq \tau \leq t} \sum_{i=1}^n \left\| \frac{\partial f_{nn}(\boldsymbol{\theta}(\tau), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} \right\|_F \int_0^t \|\boldsymbol{u}_{nn}(\tau) - \boldsymbol{y}\|_2 d\tau$$

$$\leq \frac{1}{n} \max_{0 \leq \tau \leq t} \sum_{i=1}^n \left\| \frac{\partial f_{nn}(\boldsymbol{\theta}(\tau), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} \right\|_F \int_0^t \exp\left(-\kappa^2\lambda_0\tau\right) d\tau \, \|\boldsymbol{u}_{nn}(0) - \boldsymbol{y}\|_2$$

$$\leq \frac{C_0}{\sqrt{n}\lambda_0} \max_{0 \leq \tau \leq t} \sum_{i=1}^n \left\| \frac{\partial f_{nn}(\boldsymbol{\theta}(\tau), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} \right\|_F$$

$$\leq \frac{C_0}{\sqrt{n}\kappa^2\lambda_0} \max_{0 \leq \tau \leq t} \sum_{i=1}^n \left(\left\| \frac{\partial f_{nn}(\boldsymbol{\theta}(0), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} \right\|_F + \left\| \frac{\partial f_{nn}(\boldsymbol{\theta}(\tau), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} - \frac{\partial f_{nn}(\boldsymbol{\theta}(0), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} \right\|_F \right)$$

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$$\leq \frac{C_1}{\sqrt{n}\lambda_0} \max_{0 \leq \tau \leq t} \sum_{i=1}^n \left(\left\| \frac{\partial f_{nn}(\boldsymbol{\theta}(0), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} \right\|_F + \left\| \frac{\partial f_{nn}(\boldsymbol{\theta}(\tau), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} - \frac{\partial f_{nn}(\boldsymbol{\theta}(0), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} \right\|_F \right)$$

$$\leq \frac{C_2\sqrt{n}}{\lambda_0} + \frac{C_1\sqrt{n}}{\lambda_0} \max_{0 \leq \tau \leq t} \left(\left\| \frac{\partial f_{nn}(\boldsymbol{\theta}(\tau), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} - \frac{\partial f_{nn}(\boldsymbol{\theta}(0), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} \right\|_F \right).$$

The last step we used $\left\| \frac{\partial f_{nn}(\boldsymbol{\theta}(0), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} \right\|_F = O(1)$. Suppose there exists t such that $\left\| \boldsymbol{W}^{(h)}(t) - \boldsymbol{W}^{(h)}(0) \right\|_F > \omega\sqrt{m}$. Denote

$$t_0 = \operatorname{argmin}_{t \geq 0} \left\{ \left\| \boldsymbol{W}^{(h)}(t) - \boldsymbol{W}^{(h)}(0) \right\|_F > \omega\sqrt{m}. \right\}.$$

For any $t < t_0$, we know for all $h' \in [L+1]$, $\left\| \boldsymbol{W}^{(h')}(t) - \boldsymbol{W}^{(h')}(0) \right\|_2 \leq \omega\sqrt{m}$. Therefore, by Lemma D.4, we know

$$\left\| \frac{\partial f_{nn}(\boldsymbol{\theta}(t), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} - \frac{\partial f_{nn}(\boldsymbol{\theta}(0), \boldsymbol{x}_i)}{\partial \boldsymbol{W}^{(h)}} \right\|_F = C\omega^{1/3}L^{5/2}.$$

Therefore, using the fact that ω is sufficiently small we can bound

$$\left\| \boldsymbol{W}^{(h)}(t_0) - \boldsymbol{W}^{(h)}(0) \right\|_F \leq \frac{C_3\sqrt{n}}{\lambda_0}.$$

Since we also know m is sufficiently large to make $\omega\sqrt{m} > \frac{C_3\sqrt{n}}{\lambda_0}$, we have a contradiction. $\qquad \square$

The next lemma shows if all weight matrices only have small perturbation, then we still have linear convergence.

Lemma D.6. *Suppose* $\omega = \operatorname{poly}(1/n, \lambda_0, 1/L, 1/\log(m), \epsilon, 1/\log(1/\delta), \kappa)$. *Suppose for all* $t \geq 0$ $\left\| \boldsymbol{W}^{(h)}(t) - \boldsymbol{W}^{(h)}(0) \right\|_F \leq \omega\sqrt{m}$ *for* $h \in [L+1]$. *Then if* $m = \operatorname{poly}(1/\omega)$, *we have with probability at least* $1 - \delta$ *over random initialization, for all* $t \geq 0$

$$\left\| \boldsymbol{u}_{nn}(t) - \boldsymbol{y} \right\|_2 \leq \exp\left(-\frac{1}{2}\kappa^2\lambda_0 t \right) \left\| \boldsymbol{u}_{nn}(0) - \boldsymbol{y} \right\|_2.$$

Proof of Lemma D.6. Under this assumption and the result of initialization, we know for all $t \geq 0$, $\lambda_{\min}(\boldsymbol{H}(t)) \geq \frac{1}{2}\lambda_0$. This in turn directly imply the linear convergence result we want. $\qquad \square$

Lastly, with these lemmas at hand, using an argument similar to Du et al. [2019], we can show during training, weight matrices do not move by much.

Lemma D.7. *Let* $\omega \leq \operatorname{poly}(\epsilon, L, \lambda_0, 1/\log(m), 1/\log(1/\delta), \kappa, 1/n)$. *If* $m \geq \operatorname{poly}(\omega)$, *then with probability at least* $1 - \delta$ *over random initialization, we have for all* $t \geq 0$, *for all* $h \in [L+1]$ *we have*

$$\left\| \boldsymbol{W}^{(h)}(t) - \boldsymbol{W}^{(h)}(0) \right\|_F \leq \omega\sqrt{m}$$

and

$$\left\| \boldsymbol{u}_{nn}(t) - \boldsymbol{y} \right\|_2 \leq \exp\left(-\frac{1}{2}\kappa^2\lambda_0 t \right) \left\| \boldsymbol{u}_{nn}(0) - \boldsymbol{y} \right\|_2.$$

Proof of Lemma D.7. Let

$$t_0 = \operatorname{argmin}_t \left\{ \exists h \in [L+1], \left\| \boldsymbol{W}^{(h)}(t) - \boldsymbol{W}^{(h)}(0) \right\|_F > \omega\sqrt{m} \right.$$

$$\left. \text{or } \|\boldsymbol{u}_{nn}(t) - \boldsymbol{y}\|_2 > \exp\left(-\frac{1}{2}\kappa^2\lambda_0 t\right) \|\boldsymbol{u}_{nn}(0) - \boldsymbol{y}\|_2 \right\}.$$

We analyze case by case. Suppose at time t_0, $\left\| \boldsymbol{W}^{(h)}(t_0) - \boldsymbol{W}^{(h)}(0) \right\|_F > \omega\sqrt{m}$. By Lemma D.5, we know there exists some $0 \le t_1 < t_0$ such that either there exists $h' \ne h$ such that

$$\left\| \boldsymbol{W}^{(h')}(t_1) - \boldsymbol{W}^{(h')}(0) \right\|_F > \omega\sqrt{m}$$

or

$$\|\boldsymbol{u}_{nn}(t_1) - \boldsymbol{y}\|_2 > \exp\left(-\frac{1}{2}\kappa^2\lambda_0 t_1\right) \|\boldsymbol{u}_{nn}(0) - \boldsymbol{y}\|_2.$$

However, this violates the minimality of t_0. For the other case, if

$$\|\boldsymbol{u}_{nn}(t_0) - \boldsymbol{y}\|_2 > \exp\left(-\frac{1}{2}\kappa^2\lambda_0 t_0\right) \|\boldsymbol{u}_{nn}(0) - \boldsymbol{y}\|_2,$$

By Lemma D.6, we know there exists $t_1 < t_0$ such that there exists $h \in [L+1]$,

$$\left\| \boldsymbol{W}^{(h)}(t_1) - \boldsymbol{W}^{(h)}(0) \right\|_F > \omega\sqrt{m}.$$

However, again this violates the minimality of t_0. $\qquad\square$

Now we can finish the proof of Theorem D.1.

Proof of Theorem D.1. By Lemma D.7, we know for $t \to \infty$, $\left\| \boldsymbol{W}^{(h)}(t) - \boldsymbol{W}^{(h)}(0) \right\|_F \le O\left(\omega\sqrt{m}\right)$ for if ω is sufficiently. Applying Lemma D.4, we know we only have a small perturbation on the gradient. Applying Lemma D.1, we know we only have small perturbation on kernel values. $\qquad\square$

E   CNTK Derivations

In this section we derive CNTK for formula for the vanilla CNN. Given $\boldsymbol{x} \in \mathbb{R}^{P \times Q}$ and $(i, j) \in [P] \times [Q]$, we define

$$\phi_{ij}(\boldsymbol{x}) = [\boldsymbol{x}]_{i-(q+1)/2:i+(q+1)/2, j-(q+1)/2:j+(q+1)/2}$$

i.e., this operator extracts the (i, j)-th patch. By this definition, we can rewrite the CNN definition.

CNN Definition

- Let $\boldsymbol{x}^{(0)} = \boldsymbol{x} \in \mathbb{R}^{P \times Q \times C^{(0)}}$ be the input image where $C^{(0)}$ is the number of channels in the input image.

- For $h = 1, \ldots, H$, $\beta = 1, \ldots, C^{(h)}$, the intermediate outputs are defined as

$$\left[\tilde{\boldsymbol{x}}_{(\beta)}^{(h)} \right]_{ij} = \sum_{\alpha}^{C^{(h-1)}} \left\langle \boldsymbol{W}_{(\alpha),(\beta)}^{(h)}, \phi_{ij}\left(x_{(\alpha)}^{(h-1)} \right) \right\rangle, \quad \boldsymbol{x}_{(\beta)}^{(h)} = \sqrt{\frac{c_\sigma}{C^{(h)} \times q \times q}} \sigma\left(\tilde{\boldsymbol{x}}_{(\beta)}^{(h)} \right)$$

  where each $\boldsymbol{W}_{(\alpha),(\beta)}^{(h)} \in \mathbb{R}^{q \times q}$ is a filter with Gaussian initialization.

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- The final output is defined as

$$f(\boldsymbol{\theta}, \boldsymbol{x}) = \sum_{\alpha=1}^{C^{(H)}} \left\langle \boldsymbol{W}_{(\alpha)}^{(H)}, \boldsymbol{x}_{(\alpha)}^{(H)} \right\rangle$$

where $\boldsymbol{W}_{(\alpha)}^{(H)} \in \mathbb{R}^{P \times Q}$ is a weight matrix with Gaussian initialization.

E.1 Expansion of CNTK

We expand $\Theta^{(H)}(\boldsymbol{x}, \boldsymbol{x}')$ to show we can write it as the sum of $(H + 1)$ terms with each term representing the inner product between the gradients with respect to the weight matrix of one layer. We first define an linear operator

$$\mathcal{L} : \mathbb{R}^{P \times Q \times P \times Q} \to \mathbb{R}^{P \times Q \times P \times Q}$$

$$[\mathcal{L}(\boldsymbol{M})]_{k\ell, k'\ell'} = \frac{c_\sigma}{q^2} \mathrm{tr}\left([\boldsymbol{M}]_{\mathcal{D}_{k\ell, k'\ell'}}\right). \tag{34}$$

This linear operator is induced from convolutional operation. With this operator, we can expand CNTK as (for simplicity we drop on $\boldsymbol{x}$ and $\boldsymbol{x}'$)

$$\Theta^{(H)}$$
$$= \mathrm{tr}\left(\dot{\boldsymbol{K}}^{(H)} \odot \Theta^{(H-1)} + \boldsymbol{K}^{(H)}\right)$$
$$= \mathrm{tr}\left(\boldsymbol{K}^{(H)}\right) + \mathrm{tr}\left(\dot{\boldsymbol{K}}^{(H)} \odot \mathcal{L}\left(\boldsymbol{K}^{(H-1)}\right)\right) + \mathrm{tr}\left(\dot{\boldsymbol{K}}^{(H)} \odot \mathcal{L}\left(\dot{\boldsymbol{K}}^{(H-1)} \odot \Theta^{(H-2)}\right)\right)$$
$$= \ldots$$
$$= \sum_{h=0}^{H} \mathrm{tr}\left(\dot{\boldsymbol{K}}^{(H)} \odot \mathcal{L}\left(\dot{\boldsymbol{K}}^{(H-1)} \mathcal{L}\left(\cdots \dot{\boldsymbol{K}}^{(h+1)} \mathcal{L}\left(\boldsymbol{K}^{(h)}\right) \cdots\right)\right).\right)$$

Here for $h = H$, the term is just $\mathrm{tr}\left(\boldsymbol{K}^{(H)}\right)$.

In the following, we will show

$$\mathop{\mathbb{E}}_{\boldsymbol{\theta} \sim \mathcal{W}} \left\langle \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{W}^{(h)}}, \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \boldsymbol{W}^{(h)}} \right\rangle \approx \mathrm{tr}\left(\dot{\boldsymbol{K}}^{(H)} \odot \mathcal{L}\left(\dot{\boldsymbol{K}}^{(H-1)} \mathcal{L}\left(\cdots \dot{\boldsymbol{K}}^{(h)} \mathcal{L}\left(\boldsymbol{K}^{(h-1)}\right) \cdots\right)\right)\right).$$

E.2 Derivation

We first compute the derivative of the prediction with respect to one single filter.

$$\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{W}_{(\alpha), (\beta)}^{(h)}} = \left\langle \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{x}_{(\beta)}}, \frac{\partial \boldsymbol{x}_{(\beta)}^{(h)}}{\partial \boldsymbol{W}_{(\alpha), (\beta)}^{(h)}} \right\rangle$$

$$= \sum_{(i,j) \in [P] \times [Q]} \left\langle \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{[\boldsymbol{x}_{(\beta)}^{(h)}]_{ij}}, \frac{\partial [\boldsymbol{x}_{(\beta)}^{(h)}]_{ij}}{\partial \boldsymbol{W}_{(\alpha), (\beta)}^{(h)}} \right\rangle$$

$$= \sum_{(i,j) \in [P] \times [Q]} \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{[\boldsymbol{x}_{(\beta)}^{(h)}]_{ij}} \sqrt{\frac{c_\sigma}{C^{(h)} q^2}} \sigma'\left(\left[\tilde{\boldsymbol{x}}_{(\beta)}^{(h)}\right]_{ij}\right) \phi_{ij}(\boldsymbol{x}_{(\alpha)}^{(h-1)}).$$

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With this expression, we proceed to we compute the inner product between gradients with respect to the h-th layer matrix

$$\sum_{\alpha=1}^{C^{(h-1)}} \sum_{\beta=1}^{C^{(h)}} \left\langle \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{W}_{(\alpha),(\beta)}^{(h)}}, \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \boldsymbol{W}_{(\alpha),(\beta)}^{(h)}} \right\rangle \tag{35}$$

$$= \sum_{\beta=1}^{C^{(h)}} \sum_{(i,j,i',j') \in [P]\times[Q]\times[P]\times[Q]} \frac{c_\sigma}{C^{(h)}q^2} \left(\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial [\boldsymbol{x}_{(\beta)}^{(h)}]_{ij}} \cdot \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial [\boldsymbol{x}_{(\beta)}'^{(h)}]_{i'j'}} \right) \left(\sigma'\left(\left[\tilde{\boldsymbol{x}}_{(\beta)}^{(h)} \right]_{ij} \right) \sigma'\left(\left[\tilde{\boldsymbol{x}}_{(\beta)}'^{(h)} \right]_{i'j'} \right) \right)$$

$$\cdot \left(\sum_{\alpha=1}^{C^{(h-1)}} \left\langle \phi_{ij}(\boldsymbol{x}_{(\alpha)}^{(h-1)}), \phi_{i'j'}(\boldsymbol{x}_{(\alpha)}'^{(h-1)}) \right\rangle \right).$$

Similar to our derivation to NTK, we can use the following approximation

$$\left(\sum_{\alpha=1}^{C^{(h-1)}} \left\langle \phi_{ij}(\boldsymbol{x}_{(\alpha)}^{(h-1)}), \phi_{i'j'}(\boldsymbol{x}_{(\alpha)}'^{(h-1)}) \right\rangle \right) \approx \mathrm{tr}\left(\left[\boldsymbol{K}^{(h-1)} \right]_{\mathcal{D}_{ij,i'j'}} \right).$$

Next, we tackle the term $\left(\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial [\boldsymbol{x}_{(\beta)}^{(h)}]_{ij}} \cdot \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial [\boldsymbol{x}_{(\beta)}'^{(h)}]_{i'j'}} \right)$. Notice that

$$\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \left[\boldsymbol{x}_{(\beta)}^{(h)} \right]_{ij}} = \sum_{(k,\ell) \in [P]\times[Q]} \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \left[\boldsymbol{x}_{(\gamma)}^{(h+1)} \right]_{k\ell}} \frac{\partial \left[\boldsymbol{x}_{(\gamma)}^{(h+1)} \right]_{k\ell}}{\partial \left[\boldsymbol{x}_{(\beta)}^{(h)} \right]_{ij}}.$$

and for $\gamma \in [C^{(h+1)}]$ and $(k, \ell) \in [P] \times [Q]$

$$\frac{\partial \left[\boldsymbol{x}_{(\gamma)}^{(h+1)} \right]_{k\ell}}{\partial \left[\boldsymbol{x}_{(\beta)}^{(h)} \right]_{ij}} = \begin{cases} \sqrt{\frac{c_\sigma}{C^{(h+1)}q^2}} \sigma'\left(\left[\tilde{\boldsymbol{x}}_{(\gamma)}^{(h+1)} \right]_{k\ell} \right) \left[\boldsymbol{W}_{(\beta),(\gamma)}^{(h+1)} \right]_{i-k+q-1,j-\ell+q-1} & \text{if } (i,j) \in \mathcal{D}_{k\ell} \\ 0 & \text{otherwise} \end{cases}.$$

We then have

$$\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \left[\boldsymbol{x}_{(\beta)}^{(h)} \right]_{ij}} \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \left[\boldsymbol{x}_{(\beta)}'^{(h)} \right]_{i'j'}}$$

$$= \sum_{k,\ell,k',\ell'} \frac{c_\sigma}{C^{(h+1)}q^2} \sum_{\gamma=1}^{C^{(h+1)}} \left(\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \left[\boldsymbol{x}_{(\gamma)}^{(h+1)} \right]_{k\ell}} \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \left[\boldsymbol{x}_{(\gamma)}^{('h+1)} \right]_{k'\ell'}} \right) \left(\sigma'\left(\left[\tilde{\boldsymbol{x}}_{(\gamma)}^{(h+1)} \right]_{k\ell} \right) \sigma'\left(\left[\tilde{\boldsymbol{x}}'_{(\gamma)}^{(h+1)} \right]_{k'\ell'} \right) \right)$$

$$\cdot \mathbb{1}\left\{ (i,j,i',j') \in \mathcal{D}_{k\ell,k'\ell'} \right\} \left[\boldsymbol{W}_{(\beta),(\gamma)}^{(h+1)} \right]_{i-k+q-1,j-\ell+q-1} \left[\boldsymbol{W}_{(\beta),(\gamma)}^{(h+1)} \right]_{i'-k'+q-1,j'-\ell'+q-1}$$

$$\approx \sum_{k,\ell,k',\ell'} \frac{c_\sigma}{C^{(h+1)}q^2} \sum_{\gamma=1}^{C^{(h+1)}} \left(\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \left[\boldsymbol{x}_{(\gamma)}^{(h+1)} \right]_{k\ell}} \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \left[\boldsymbol{x}_{(\gamma)}^{('h+1)} \right]_{k'\ell'}} \right) \left(\sigma'\left(\left[\tilde{\boldsymbol{x}}_{(\gamma)}^{(h+1)} \right]_{k\ell} \right) \sigma'\left(\left[\tilde{\boldsymbol{x}}'_{(\gamma)}^{(h+1)} \right]_{k'\ell'} \right) \right)$$

$$\cdot \mathbb{1}\left\{ (i,j,i',j') \in \mathcal{D}_{k\ell,k'\ell'}, i-k = i'-k', j-\ell = j'-\ell' \right\} \tag{36}$$

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where the last approximation is due to our initialization of $\boldsymbol{W}^{(h+1)}$. Note interestingly, this approximation shows the inner product does NOT depend on β. Using this observation, we can sum over (β) and obtain the following approximation.

$$\frac{c_\sigma}{C^{(h)}q^2} \sum_{\beta=1}^{C^{(h)}} \sigma'\left(\left[\tilde{\boldsymbol{x}}_{(\beta)}^{(h)}\right]_{ij}\right) \sigma'\left(\left[\tilde{\boldsymbol{x}}_{(\beta)}^{'(h)}\right]_{i'j'}\right) \approx \left[\dot{\boldsymbol{K}}^{(h)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right]_{ij,i'j'}.$$

Now we put everything together. For notation convenience, we define $\boldsymbol{G}^{(h),(h)}\left(\boldsymbol{x}, \boldsymbol{x}'\right) \in \mathbb{R}^{[P] \times [Q] \times [P] \times [Q]}$

$$\left[\boldsymbol{G}^{(h),(h)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right]_{ij,i'j'} = \mathrm{tr}\left(\left[\boldsymbol{K}^{(h-1)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right]_{\mathcal{D}_{ij,i'j'}}\right) \left[\dot{\boldsymbol{K}}^{(h)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right]_{ij,i'j'}.$$

We further define

$$\left[\boldsymbol{G}^{(h),(h+1)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right] = \dot{\boldsymbol{K}}^{(h+1)}(\boldsymbol{x}, \boldsymbol{x}') \odot \mathcal{L}\left(\boldsymbol{G}^{(h),(h)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right),$$

$$\left[\boldsymbol{G}^{(h),(h+2)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right] = \dot{\boldsymbol{K}}^{(h+2)}(\boldsymbol{x}, \boldsymbol{x}') \odot \mathcal{L}\left(\boldsymbol{G}^{(h),(h+1)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right),$$

$$\dots,$$

$$\left[\boldsymbol{G}^{(h),(H)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right] = \dot{\boldsymbol{K}}^{(H)}(\boldsymbol{x}, \boldsymbol{x}') \odot \mathcal{L}\left(\boldsymbol{G}^{(h),(H-1)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right).$$

Equation (35) can be written as

$$\sum_{\alpha=1}^{C^{(h-1)}} \sum_{\beta=1}^{C^{(h)}} \left\langle \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{W}_{(\alpha),(\beta)}^{(h)}}, \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \boldsymbol{W}_{(\alpha),(\beta)}^{(h)}} \right\rangle$$

$$\approx \sum_{i,j,i',j'} \left(\frac{f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \left[\boldsymbol{x}_{(\beta)}^{(h)}\right]_{ij}} \frac{f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \left[\boldsymbol{x}_{(\beta)}^{'(h)}\right]_{i'j'}}\right) \mathrm{tr}\left(\left[\boldsymbol{K}^{(h-1)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right]_{\mathcal{D}_{ij,i'j'}}\right) \left[\dot{\boldsymbol{K}}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right]_{ij,i'j'}$$

$$= \sum_{i,j,i',j'} \left(\frac{f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \left[\boldsymbol{x}_{(\beta)}^{(h)}\right]_{ij}} \frac{f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \left[\boldsymbol{x}_{(\beta)}^{'(h)}\right]_{i'j'}}\right) \left[\boldsymbol{G}^{(h),(h)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right]_{i,j,i',j'} \tag{37}$$

To proceed, we use Equation (36) to rewrite the inner product

$$\sum_{\alpha=1}^{C^{(h-1)}} \sum_{\beta=1}^{C^{(h)}} \left\langle \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \boldsymbol{W}_{(\alpha),(\beta)}^{(h)}}, \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \boldsymbol{W}_{(\alpha),(\beta)}^{(h)}} \right\rangle$$

$$\approx \sum_{k,\ell,k',\ell'} \left(\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \left[\boldsymbol{x}_{(\gamma)}^{(h+1)}\right]_{k\ell}} \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \left[\boldsymbol{x}_{(\gamma)}^{'(h+1)}\right]_{k'\ell'}}\right) \cdot \frac{c_\sigma}{C^{(h+1)}q^2} \left(\sigma'\left(\left[\tilde{\boldsymbol{x}}_{(\gamma)}^{(h+1)}\right]_{k\ell}\right) \sigma'\left(\left[\tilde{\boldsymbol{x}'}_{(\gamma)}^{(h+1)}\right]_{k'\ell'}\right)\right)$$

$$\cdot \sum_{i,j,i',j'} \mathbb{1}\left\{(i,j,i',j') \in \mathcal{D}_{k\ell,k'\ell'}, i-k = i'-k', j-\ell = j'-\ell'\right\} \left[\boldsymbol{G}^{(h),(h)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right]_{i,j,i',j'}.$$

$$\approx \sum_{k,\ell,k',\ell'} \left(\frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x})}{\partial \left[\boldsymbol{x}_{(\gamma)}^{(h+1)}\right]_{k\ell}} \frac{\partial f(\boldsymbol{\theta}, \boldsymbol{x}')}{\partial \left[\boldsymbol{x}_{(\gamma)}^{'(h+1)}\right]_{k'\ell'}}\right) \left[\boldsymbol{G}^{(h),(h+1)}\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right]_{k\ell,k'\ell'} \tag{38}$$

where in the last line's approximation, we use the definition of $\mathbf{G}^{(h),(h+1)}$ and

$$\frac{c_\sigma}{C^{(h+1)}q^2}\left(\sigma'\left(\left[\tilde{\boldsymbol{x}}_{(\gamma)}^{(h+1)}\right]_{k\ell}\right)\sigma'\left(\left[\tilde{\boldsymbol{x}}'^{(h+1)}_{(\gamma)}\right]_{k'\ell'}\right)\right)\approx\left[\dot{\boldsymbol{K}}^{(h+1)}(\boldsymbol{x},\boldsymbol{x}')\right]_{k\ell,k'\ell'}.$$

Comparing this Equation (38) with Equation (37), we now have an iterative formula. Applying this formula iteratively, we have

$$\sum_{\alpha=1}^{C^{(h-1)}}\sum_{\beta=1}^{C^{(h)}}\left\langle\frac{\partial f(\boldsymbol{\theta},\boldsymbol{x})}{\partial\boldsymbol{W}_{(\alpha),(\beta)}^{(h)}},\frac{\partial f(\boldsymbol{\theta},\boldsymbol{x}')}{\partial\boldsymbol{W}_{(\alpha),(\beta)}^{(h)}}\right\rangle$$

$$\approx\sum_{i,j,i',j'}\left(\frac{f(\boldsymbol{\theta},\boldsymbol{x})}{\partial\left[\boldsymbol{x}_{(\beta)}^{(h)}\right]_{ij}}\frac{f(\boldsymbol{\theta},\boldsymbol{x}')}{\partial\left[\boldsymbol{x}_{(\beta)}^{'(h)}\right]_{i'j'}}\right)\left[\mathbf{G}^{(h),(h)}\right]_{i,j,i',j'}$$

$$\approx\sum_{k,\ell,k',\ell'}\left(\frac{\partial f(\boldsymbol{\theta},\boldsymbol{x})}{\partial\left[\boldsymbol{x}_{(\gamma)}^{(h+1)}\right]_{k\ell}}\frac{\partial f(\boldsymbol{\theta},\boldsymbol{x}')}{\partial\left[\boldsymbol{x}_{(\gamma)}^{('h+1)}\right]_{k'\ell'}}\right)\left[\mathbf{G}^{(h),(h+1)}\right]_{k\ell,k'\ell'}$$

$$\cdots$$

$$\approx\sum_{k,\ell,k',\ell'}\left(\frac{\partial f(\boldsymbol{\theta},\boldsymbol{x})}{\partial\left[\boldsymbol{x}_{(\gamma)}^{(H)}\right]_{k\ell}}\frac{\partial f(\boldsymbol{\theta},\boldsymbol{x}')}{\partial\left[\boldsymbol{x}_{(\gamma)}^{('H)}\right]_{k'\ell'}}\right)\left[\mathbf{G}^{(h),(H)}\right]_{k\ell,k'\ell'}$$

$$\approx\sum_{k,\ell}\left(\frac{\partial f(\boldsymbol{\theta},\boldsymbol{x})}{\partial\left[\boldsymbol{x}_{(\gamma)}^{(H)}\right]_{k\ell}}\frac{\partial f(\boldsymbol{\theta},\boldsymbol{x}')}{\partial\left[\boldsymbol{x}_{(\gamma)}^{('H)}\right]_{k\ell}}\right)\left[\mathbf{G}^{(h),(H)}\right]_{k\ell,k\ell}$$

$$=\mathrm{tr}\left(\mathbf{G}^{(h),(H)}\right)$$

$$=\mathrm{tr}\left(\dot{\boldsymbol{K}}^{(H)}\odot\mathcal{L}\left(\dot{\boldsymbol{K}}^{(H-1)}\mathcal{L}\left(\cdots\dot{\boldsymbol{K}}^{(h)}\mathcal{L}\left(\boldsymbol{K}^{(h-1)}\right)\cdots\right)\right)\right).$$

The last approximation is due to the fact that we use a fully-connected weight matrix as the last layer and if $(k,\ell)\neq(k',\ell')$, the expectation is 0.