Abstract

Yang (2020a) recently showed that the Neural Tangent Kernel (NTK) at initialization has an infinite-width limit for a large class of architectures including modern staples such as ResNet and Transformers. However, their analysis does not apply to training. Here, we show the same neural networks (in the so-called NTK parametrization) during training follow a kernel gradient descent dynamics in function space, where the kernel is the infinite-width NTK. This completes the proof of the architectural universality of NTK behavior. To achieve this result, we apply the Tensor Programs technique: Write the entire SGD dynamics inside a Tensor Program and analyze it via the Master Theorem. To facilitate this proof, we develop a graphical notation for Tensor Programs.

1. Introduction

Jacot et al. (2018)’s pioneering work showed that a multilayer perceptron (MLP) trained by gradient descent (GD) evolves like a linear model. This spurred a flurry of research papers using this insight to tackle the core questions in deep learning theory, from optimization to generalization in both finite and infinite width regimes. (Jacot et al., 2018)’s argument consists of two observations:

\[ \text{NTK\textsubscript{INIT}} \quad \text{For the output of a network } f(\xi; w) \text{ with parameters } w \text{ given example } \xi, \text{ (Jacot et al., 2018) identified the kernel } K(\xi, \xi) = \langle \nabla f(\xi; w), \nabla f(\xi, w) \rangle, \text{ known as the Neural Tangent Kernel (NTK). They showed that if } f \text{ is parametrized and initialized appropriately, then } K \text{ converges to a deterministic kernel } \bar{K} \text{ as the width of the network tends to infinity.} \]

\[ \text{NTK\textsubscript{TRAIN}} \quad \text{As the infinitely wide network is trained by gradient descent, the NTK remains frozen in its initial state, and the network evolves as by kernel gradient descent with kernel } \bar{K}. \]

In (Yang, 2020a), the NTK\textsubscript{INIT} property was proven to hold for standard architectures, meaning any composition of MLPs, recurrent neural networks (RNN), LSTMs (Hochreiter & Schmidhuber, 1997), gated recurrent unit (GRU) (Cho et al., 2014), convolutions (Fukushima, 1980; 1975; Lecun et al., 1998; 2000; Rumelhart et al., 1986), residual connections (He et al., 2016; Huang et al., 2017), batch normalization (Ioffe & Szegedy, 2015), graph neural networks (Bruna et al., 2014; Defferrard et al., 2016; Duvenaud et al., 2015; Henaff et al., 2015; Kipf & Welling, 2017) and attention (Bahdanau et al., 2015; Vaswani et al., 2017), along with arbitrary weight sharing between components. More generally, it holds for any architecture expressible in a so-called Tensor Program (Yang, 2019b;a; 2020a;b), of which the standard architectures are a subset. However, their reasoning is limited to initialization only.

A statement is architecturally universal if it holds for any reasonable neural architecture. This is an informal property, but here we will formalize it by taking reasonable to be “expressible in Tensor Programs.” By the expressiveness of such programs (Yang, 2019a; 2020a), architectural universality is a fairly robust notion that covers present (and, we expect, future) architectures comprehensively. In this terminology, (Yang, 2020a) showed that NTK\textsubscript{INIT} is architecturally universal.

Our Contribution We show the architectural universality of the entire NTK theory by proving NTK\textsubscript{TRAIN} for the same architectures discussed above, including all standard architectures. In the process, we introduce a new graphical form of Tensor Programs that is both required in our proofs and useful for the pedagogy of Tensor Programs.

The Tensor Program Series This paper follows (Yang, 2019b;a; 2020a;b; Yang & Hu, 2020) in the series. While we number this paper “IIb” right after (Yang, 2020a), we actually need the complete theoretical foundation developed in III (Yang, 2020b). See Footnote 22 for more details.

2. Background

Let \( f(\xi; w) \in \mathbb{R} \) denote the (scalar) output of a neural network parameterized by \( w \), given example \( \xi \). To understand how the output changes with a slight change in the network
parameters $w_0 - \delta w$, we may naively expand the network function using the first order Taylor expansion around a base point $w_0$:

$$f(\xi, w_0 - \delta w) - f(\xi; w_0) \approx \langle \nabla_w f(\xi, w_0), \delta w \rangle.$$  \hspace{1cm} (1)

Under the SGD algorithm, the weight update $\delta w$ is given by the gradient $\delta w = -\eta \chi(\hat{\xi}) \nabla_w f(\xi; w_0)$ where $\chi(\xi)$ is the loss derivative, $\hat{\xi}$ is a sample from the training set, and $\eta$ is the learning rate. Plugging into Eq. (1), we get:

$$f(\xi, w_0 - \delta w) - f(\xi; w_0) \approx -\eta \chi(\hat{\xi}) K(\xi, \hat{\xi}).$$  \hspace{1cm} (2)

where $K(\xi, \hat{\xi}) = \langle \nabla_w f(\xi; w_0), \nabla_w f(\hat{\xi}; w_0) \rangle$ is the NTK. The NTK theory of infinitely wide neural networks as first proposed by (Jacot et al., 2018) boils down to the following observations: *When the width of $f$ tend to infinity, the NTK $K$ converges to a fixed kernel $\hat{K}$ at random initialization, independent of the specific instantiation of the weights, and remains frozen during the optimization process.* Eq. (2) then gives an accurate description of the output evolution with it we substitute $K$ with $\hat{K}$. The seemingly complex optimization trajectory of SGD therefore reduce to the convex trajectory of kernel gradient descent with a time-independent kernel $\hat{K}$.

Consider the output of the network $f \in \mathbb{R}^D$ on the full training dataset. As shown in (Jacot et al., 2018), when the $L2$ loss is used the evolution of the output $f_t$ at time $t$ under continuous time GD (i.e. gradient flow) takes a simple form:

$$f_t - f^* = e^{-\eta \hat{K}_t}(f_0 - f^*).$$

where $\hat{K} \in \mathbb{R}^{D \times D}$ is the full NTK matrix evaluated on the training data, $f^*$ is the label function, and $f_0$ is the output at initialization. Hence, provided $\hat{K}$ is full rank, as $t \to \infty$ we have that $f_t \to f^*$, and the network can fit the training data perfectly.

**Previous Approaches vs Ours** A common theme in showing NTKTrain for MLP is to derive high-probability bounds on the deviation of the NTK $K$ from its initial value after training (e.g. Allen-Zhu et al. (2018); Du et al. (2018); Zou et al. (2018)). Obtaining these bounds usually requires developing ad hoc methods on a per-architecture basis, hindering the scalability of the method to other settings. In the present work we take a more holistic approach, leveraging the recently developed Tensor Programs framework (Yang, 2019b;a; 2020a,b). It consists of two layers of arguments: 1) The bottom layer analyzes how the distribution of pre-activations change throughout the course of training; this crucially leverages the mathematical machinery of the Tensor Programs Master Theorem. 2) The top layer packages these insights systematically via the notion of paths so as to apply to any architecture expressible by a Tensor Program. We will illustrate 1) through examples in Section 3 and 2) through figures in Section 5.1.

**Setup and Notations** In this paper, we will consider the architecture (including depth), data, and training time to be fixed as $n \to \infty$. We describe common notations used in the remainder of the paper. For simplicity, we will consider SGD with batch size 1 and learning rate $\eta$ (often set to 1 WLOG). We use $\xi_t$ to denote the input and $L_t$ to denote the loss function (absorbing the label) at step $t$. More generally, subscript $t$ on any symbol means time $t$. However, for brevity, we abuse notation and shorthand $f_t$ for $f_t(\xi_t)$, and, for any (pre-)activation $x$, $x_t$ for $x_t(\xi_t)$. We will also write $\chi_t$ for the loss derivative $L_t'(f_t)$. For any vector $v(\xi)$ we define $\delta v_{t+1}(\xi) \triangleq \sqrt{n}(x_{t+1}(\xi) - x_t(\xi))$ and $dx(\xi) \triangleq \sqrt{n} \frac{\partial f(\xi)}{\partial \xi}$. We will track the evolution of $f$ on an arbitrary input $\xi$. Similar to above, we shorthand $\hat{x}_t, \hat{f}_t$ for $x_t(\hat{\xi}), f_t(\hat{\xi})$.

### 3. Motivating Examples

The purpose of this section is to illustrate our key ideas via simple, intuitive examples without diving into the specifics of Tensor Programs. In the process, we will gain insight into how randomness from initialization propagates over the course of training. As these examples intend to provide the reader with the proper intuition, we use informal arguments alone and relegate all formal statements to the appendix. For brevity, we will gloss over minor details or routine calculations, but interested readers can see Appendix A for these omissions.

**Key Idea** It turns out that the random initialization and the overparametrization of weights cause each (pre-)activation vector $x_t(\xi) \in \mathbb{R}^n$, its gradient $dx_t(\xi) \in \mathbb{R}^n$, and its (scaled) change $\delta x_t(\xi) \in \mathbb{R}^n$ every time step $t$ to have roughly iid coordinates, not just initially but throughout training. Then, as we shall demonstrate through the examples below, to track the evolution of the neural network function, it suffices to track the evolution of the coordinate distributions of $x(\xi)$, $dx(\xi)$, $\delta x(\xi)$. We write $Z^{x(\xi)}, Z^{dx(\xi)}, Z^{\delta x(\xi)} \in \mathbb{R}$ for the random variables corresponding to such coordinate distributions.

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1. In the original NTK paper (Jacot et al., 2018), the limit is taken as each layer width goes to infinity sequentially, which already doesn’t make sense for weight-tied architectures like RNNs.
2. In particular, we need to use the Master Theorem in (Yang, 2020b), so (Yang, 2020a) could not have obtained NTKTrain at the same time as NTKInit.

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3. They will affect the rate of convergence to the infinite-width limit, but since we are only concerned with whether convergence occurs, they do not appear in our theorem statements here.
4. This generalizes readily to any batch size and learning rate.
5. We will not refer to the function $x_t : \xi \to x_t(\xi)$ (likewise for $f_t, \chi_t$), so this abuse of notation should cause no confusion.
6. It might help to think of $\xi$ as some test sample, but it can also fall in the training set.
7. This is a consequence of the Tensor Program Master Theorem.
8. As we will explain below, different $Z$’s may correlate, reflecting correlations between corresponding vectors.
Our goal is to derive, from these insights,

**Claim 3.1.** In the large width limit, \( \tilde{f}_t = f_t(\tilde{\xi}) \) changes by

\[
\lim_{n \to \infty} \tilde{f}_{t+1} - \tilde{f}_t = -\tilde{\chi}_t \tilde{K}(\tilde{\xi}, \xi_t) \tag{3}
\]

at step \( t \), where \( \tilde{K} \) is the limiting NTK of the architecture and \( \tilde{\chi}_t = \mathcal{L}_t'(\lim_n f_t) \) is the loss derivative.

We start with an example derivation for 1-hidden-layer MLP, before moving on to 2-hidden-layers, where the mathematics quickly become much more involved.

### 3.1. 1 Hidden Layer

Consider a 1-hidden-layer network with nonlinearity \( \phi \):

\[
f = V^T x, \quad x = \phi(h), \quad h = U \xi
\]

where \( \xi \in \mathbb{R}^d, U = \frac{n}{\sqrt{d}} \in \mathbb{R}^{n \times d}, V = \frac{1}{\sqrt{n}} \in \mathbb{R}^{n \times 1}, \) for trainable parameter tensor \( u \), initialized iid from \( \mathcal{N}(0, 1) \). In the interest of clarity we assume the output layer is not trained, and \( d = 1 \).

For a vector \( v \in \mathbb{R}^n \), let \( v = \Theta(n^a) \) mean that “\( v \) has coordinates of order \( n^a \) when \( n \) is large”; likewise for \( o(n^a) \), etc. Recall the notations \( x_t = x_t(\xi_t), \tilde{x}_t = x_t(\tilde{\xi}), \delta x_t = \sqrt{n}(x_t - x_{t-1}) \) and likewise for \( h_t, \hat{h}_t, \delta h_t \). The key insights are as follows:

#### Preliminary Calculations

It turns out \( \tilde{x}_{t+1} - \tilde{x}_t = \Theta(1/\sqrt{n}) = o(1) \) so \( \delta \tilde{x}_{t+1} = \sqrt{n}(\tilde{x}_{t+1} - \tilde{x}_t) \) has \( \Theta(1) \) coordinates. Likewise for \( \delta \hat{h}_{t+1} \). Consequently, for any \( t \) and input \( \xi \), by telescoping,

\[
h_t(\xi) = h_0(\xi) + o(1). \tag{4}
\]

Using \( \nabla_u f = \frac{1}{\sqrt{n}} d h_t \xi_t^\top \) and \( dh_k = \phi'(h_t) \odot v \), we have:

\[
\delta \hat{h}_{t+1} = -\tilde{\chi}_t \xi_t^\top \tilde{\xi} \phi'(h_t) \odot v. \tag{5}
\]

Also, \( \delta \tilde{x}_{t+1} = \sqrt{n}(\phi(\tilde{h}_t + \delta \tilde{h}_{t+1}) - \phi(\tilde{h}_t)) \). Since \( \delta \tilde{h}_{t+1} = \Theta(1) \), by intuitive Taylor expansion, we have

\[
\delta \tilde{x}_{t+1} \approx \phi'(\tilde{h}_t) \odot \delta \hat{h}_{t+1}. \tag{6}
\]

The change in the output on example \( \tilde{\xi} \) from step \( t \) to step \( t + 1 \) is given by:

\[
\tilde{f}_{t+1} - \tilde{f}_t = V^T (\tilde{x}_{t+1} - \tilde{x}_t) = v^\top \delta \tilde{x}_{t+1} / n \tag{7}
\]

#### IID Coordinates

By definition \( v \) has iid coordinates. It turns out \( h_t(\xi), \delta h_t(\xi) \) (likewise for \( x \) all have approx. iid coordinates of size \( \Theta(1) \) as well.\(^{10}\) Let \( Z^{\delta \tilde{x}_t}, Z^v \) denote the random variables encoding the corresponding coordinate distributions; likewise for the other vectors. Note that \( Z^{\delta \tilde{x}_t}, Z^v \) will in general be correlated, reflecting the coordinatewise correlation between \( v \) and \( \delta \tilde{x}_t \).

#### Law of Large Numbers

and Eqs. (5) and (7) imply,

\[
\lim_{n \to \infty} \tilde{f}_{t+1} - \tilde{f}_t = \mathbb{E} Z^v Z^{\delta \tilde{x}_{t+1}} \tag{8}
\]

\[
= -\tilde{\chi}_t \xi_t^\top \tilde{\xi} \mathbb{E} \phi'(Z^{\hat{h}_t}) \phi'(Z^{\hat{h}_t})(Z^v)^2. \tag{9}
\]

where \( \tilde{\chi}_t = \mathcal{L}_t'(\lim_n f_t) \) as in Claim 3.1.

#### Kernel Expression as Gaussian Expectation

By Eq. (4), in the \( n \to \infty \) limit, \( Z^{\hat{h}_t} = Z^{h_0(\xi)} \) and \( Z^{\hat{h}_t} = Z^{h_0(\xi_t)} \), they are independent from \( Z^v \) and jointly Gaussian with variances \( \|\xi\|^2, \|\xi_t\|^2 \) and covariance \( \xi^\top \xi_t \). So (using the initialization of \( v \) to simplify \( \mathbb{E}(Z^v)^2 = 1 \)),

\[
\lim_{n \to \infty} \tilde{f}_{t+1} - \tilde{f}_t = -\tilde{\chi}_t \xi_t^\top \tilde{\xi} \mathbb{E} \phi'(Z^{h_0(\xi)}) \phi'(Z^{h_0(\xi)}). \tag{10}
\]

This can easily be seen to be Eq. (3) (recall we assumed for simplicity the output layer \( V \) is not trained).

#### Summary

Our strategy so far has been computing the form of \( Z^{\delta \tilde{x}_t} \) and plugging it into Eq. (8) to compute the dynamics of the output in the limit. Note that our approach differs from previous work which mainly focus on proving a bound on the change of the NTK post training. As the architecture gets more complex, bounding the NTK movement becomes quite complex, but our approach easily scales due to the automation provided by the Tensor Programs framework (see Section 4).

In the previous example, the coordinate distribution \( Z^{\tilde{x}_t} \) took a fairly simple form, which allowed us to intuitively compute the expectation \( \mathbb{E} Z^{\delta \tilde{x}_t} Z^v \). Before introducing a method for computing coordinate distributions in a general architecture, we move on to a slightly more involved architecture, with the intention of highlighting the intuition behind the general case.

### 3.2. 2 Hidden Layers

In this example we consider a model of the form:

\[
f = V^T x, \quad x = \phi(h), \quad h = Wz
\]

\[
z = \phi(g), \quad g = U \xi
\]

where \( U = \frac{u}{\sqrt{d}} \in \mathbb{R}^{n \times d}, W = \frac{u}{\sqrt{n}} \in \mathbb{R}^{n \times n}, V = \frac{1}{\sqrt{n}} \in \mathbb{R}^{n \times 1}, \) for trainable parameters \( u, w, \) initialized iid from a

\(^{10}\)Technically, they have iid coordinates only after conditioning on the initial function (GP) \( f_0 \). Likewise, when we take expectation in this example (e.g. Eqs. (9) and (17)), it’s a conditional expectation of this kind. See Appendix D.1.1 for a rigorous treatment. However, to convey the main intuition, we gloss over this technicality here.
normal distribution. As before we assume the last layer is not trained, and \( d = 1 \).

Again, we want to establish Claim 3.1 for this model. As in the 1-hidden-layer example, the dynamics of the output in the limit is still given by Eq. (8). This time around, the second hidden layer adds nontrivial complexity when evaluating the expectation \( \mathbb{E} Z^\alpha Z^{\delta z_{t+1}} \). As we shall see, this complexity arises from the dependency of \( \hat{x} \) on the \( n \times n \) matrices \( w \) and \( w' \), which will make it wrong to naively apply LLN arguments. Resolving this complexity will pave the way to a general strategy which we will then be able to apply in any arbitrary architecture. We now apply the same insights as in the 1-hidden-layer MLP. Namely:

- Eq. (4) continues to hold with \( h \) replaced by any of \( \{x, h, z, g\} \).
- After some brief calculations, with \( d_h \) denoting the scaled gradient \( \sqrt{n} \nabla_h f \),
  \[ \delta \hat{y}_{t+1} \approx -\chi t \xi_t^\top \xi' (g_t) \odot (W^\top d_h) \]  
  \[ \delta \tilde{h}_{t+1} \approx W \delta \tilde{z}_{t+1} - \chi_t \xi_t^\top \xi' (h_t) \odot v. \]  
- As in the 1-hidden-layer case, for all \( x \in \{g, z, h, x\} \), \( x_t(\xi) \), \( \delta x_t(\xi) \) have iid coordinates of size \( \Theta(1) \), as does \( v \) by definition.\(^{11} \) Let \( Z^{\delta x}, Z^{\delta z} \) denote the (generally correlated) random variables encoding the corresponding coordinate distributions.
- As in Eq. (7), by naive Taylor expansion we have:
  \[ \delta \tilde{z}_{t+1} \approx \phi'(\hat{y}_t) \odot \delta \hat{y}_{t+1}. \] 
- Eqs. (6) and (7) in the 1-hidden-layer case continue to hold here. Then by Eq. (12) and Law of Large Numbers,
  \[ \lim_{n \to \infty} \tilde{f}_{t+1} - \tilde{f} = \mathbb{E} Z^\alpha Z^{\delta \tilde{z}_{t+1}} \]  
  \[ = -\chi_t \xi_t^\top \xi \mathbb{E}[Z^\alpha Z^\delta] \mathbb{E}[\phi'(Z^\delta h_t)] + Z^\delta Z^{\delta \tilde{z}_{t+1}} Z^\alpha. \]  
where \( \chi_t = \mathcal{O}(\text{lim}_n f_t) \) as in Claim 3.1.

In this expression, the first term (Eq. (15)) can easily be seen to correspond to the contribution from \( w \) to the NTK. It remains to show that the second (Eq. (16)) corresponds to the contribution from \( u \).

Challenge of Analyzing Eq. (16) To do this, we must reason about the coordinate distribution of \( W \delta \tilde{z}_{t+1} \) (encoded by random variable \( Z^W \delta \tilde{z}_{t+1} \)) and compute the expectation in Eq. (16). To understand why this represents a greater challenge than it might first appear, note that from \( \delta \tilde{z}_{t+1} \approx \phi'(\hat{y}_t) \odot \delta \hat{y}_{t+1} \) (Eq. (13)), the term \( W \delta \tilde{z}_{t+1} \) hides within itself a dependency on \( W^\top d_h \) through \( \delta \hat{y} \) (Eq. (11)).

While at \( t = 0 \), we may assume \( W^\top \) is independent of \( W \) and obtain the correct results (Gradient Independent Assumption (Yang & Schoenholz, 2017; Yang, 2020a)), this is no longer the case for \( t > 0 \): \( Z^W \delta \tilde{z}_{t+1} \) will be nontrivially correlated with \( \phi'(Z^h_t) \) and \( Z^u \) (which would be false if \( W^\top \) can be assumed independent of \( W \)). We will give some intuition why later in Eq. (20). Now, what is this dependence exactly?

Claim 3.2. Based on the above discussion and some easy calculations, \( \delta \tilde{z}_{t+1} \) can be written as \( \Phi(W^\top d_h) \) for some \( \Phi : \mathbb{R} \to \mathbb{R} \) applied coordinatewise (which will depend on other vectors not of the form \( W^\top \)). Then it turns out\(^{11} \)

\[ Z^W \delta \tilde{z}_{t+1} = G + Z^{dh} \mathbb{E} \frac{\partial Z\delta \tilde{z}_{t+1}}{\partial Z^W} d_h, \]  
where \( G \) is some Gaussian variable independent from \( Z^u \), and \( \mathbb{E} \frac{\partial Z\delta \tilde{z}_{t+1}}{\partial Z^W} d_h = \Phi'(Z^{W^\top} d_h) \).

Getting Claim 3.1 Thus, from Eqs. (11) and (13), it follows that:

\[ Z^{\delta \tilde{z}_{t+1}} = -\chi_t \xi_t^\top \xi \mathbb{E}[\phi'(Z^\delta h_t)] Z^{W^\top} d_h + \mathbb{E} \frac{\partial Z\delta \tilde{z}_{t+1}}{\partial Z^W} d_h = -\chi_t \xi_t^\top \xi \mathbb{E}[\phi'(Z^\delta h_t)] Z^{W^\top} d_h, \]

Plugging into Eqs. (14) and (17), followed by some straightforward calculation, then yields Claim 3.1.

Intuition behind Claim 3.2 Eq. (17) may appear cryptic at first, so let’s give some intuition using an example. Suppose \( \Phi \) in Claim 3.2 is actually identity. For brevity, we set \( x = d_h, y = \delta \tilde{z}_{t+1} \in \mathbb{R}^n \). Then, following straightforward calculation, \( W y = W^\top x \) has coordinates

\[ (Wy)_\alpha = \sum_{\gamma \beta} x_\gamma \sum_{\beta=1}^n W_{\alpha \beta} W_{\gamma \beta} + \sum_{\beta=1}^n (W_{\alpha \beta})^2 x_\alpha \]  
Now, the second sum converges via LLN to \( x_\alpha \) as \( n \to \infty \). On the other hand, the first sum will converge via CLT to \( N(0, \lim \|x\|^2/n) \). Thus, in terms of \( Z_s \), we have

\[ Z^W y = G + Z^x = G + Z^x \mathbb{E} \Phi' \]

for some Gaussian \( G \); this corresponds directly to Eq. (17).\(^{12} \)

For general \( \Phi \), a similar intuition applies after Taylor expansion of \( \Phi \).

\(^{11}\)This example was worked out in (Yang, 2020a; b) as well, though in different contexts. Readers needing more explanation may see those works.
Figure 1: Graphical form of NetTOR{T} programs for MLP and RNN. An empty node corresponds to a G-var (an initial vector or a vector created by MatMul), while a filled node corresponds to an X-var (a vector created by Nonlin). Each dashed edge corresponds to matrix multiplication by the labeled matrix. Each gate (connected by solid edges) represents a Nonlin application. The computation follows the direction of the gates (left-to-right here). Note we have \( W^3 \xi \) instead of \( \xi \) as an initial vector because we only allow \( \mathbb{R}^3 \) vectors; likewise for \( U \xi \). For the same reason, we don’t express the network output in this graph.

Summary

This 2-hidden-layer example proceeded much the same as the 1-hidden-layer case, with the main exception of analyzing the interaction of the \( n \times n \) Gaussian matrix \( W \) and \( W^T \) (Eq. (16)) that occurs after taking at least 1 step of SGD. This was absent in the 1-hidden-layer case because each weight matrix has at most one side tending to infinity. Such analysis is crucial to obtaining the right results, as assuming \( W^T \) be independent from \( W \) would imply \( f \) does not move from initialization.\(^{13}\)

It turns out these two examples have essentially covered all of the core ideas needed to extend the analysis into arbitrary architectures. To formalize and scale up our calculations, we now turn to the Tensor Programs framework.

4. Tensor Programs

So far, our results have been obtained by unrolling the SGD updates on toy models with specific architectures, and using informal arguments. Obviously, these computations quickly become unmanageable when the architecture becomes more complex. The sheer amount of architectural innovations that have sprung up in recent years requires us to adopt a much more general formulation of our results. To that end, we adopt the Tensor Programs (TP) framework developed in (Yang, 2019a; 2020a,b). In a nutshell, it provides a language for describing typical computations done in the context of neural networks, such as forward and backward propagation. It is simultaneously simple and expressive, covering all standard architectures (Yang, 2019a; 2020a). Here we review two basic forms of Tensor Programs, NetTOR{T} and NetTOR{T}+.

**Definition 4.1.** A NetTOR{T} program is just a sequence of \( \mathbb{R}^n \) vectors inductively generated via one of the following instructions from an initial set \( V \) of random \( \mathbb{R}^n \) vectors and a set \( W \) of random \( n \times n \) matrices

\[
\text{NONLIN} \quad \text{For } x^1, \ldots, x^k \in \mathbb{R}^n \text{ in the program and any } \\
\psi : \mathbb{R}^k \to \mathbb{R}, \text{ we can generate } \psi(x^1, \ldots, x^k) \in \mathbb{R}^n
\]

\[
\text{MATMUL} \quad \text{Given } W \in \mathbb{R}^{n \times n} \text{ and } x \in \mathbb{R}^n, \text{ we can generate } W x \in \mathbb{R}^n \text{ or } W^T x \in \mathbb{R}^n
\]

**Graphical Form** We propose to represent a NetTOR{T} program as a computational graph, where each node in the graph represents vectors (initial or generated), each (dashed) edge represents a MatMul, and each gate represents a Nonlin. For example, Fig. 1 shows the computation graphs expressing (the forward passes of) an MLP and an RNN. We can also express the backpropagation as well (see Fig. 6). Graphically, the initial vectors are the empty nodes with only one edge coming out, toward the direction of computation. The matrices correspond to (the labels of) the dashed edges. We can also define the output vectors to correspond to the nodes that have only one edge coming out, against the direction of computation.

**Neural Network Representation** Each NetTOR{T} program can be thought of as computing a function \( (\mathbb{R}^n)^V \times (\mathbb{R}^{n \times n})^W \to \mathbb{R}^n \) taking an instantiation of the initial vectors \( V \) and matrices \( W \) and computing the values of all output vectors \( \mathcal{Y} \). We can say a program represents a network if it computes the body of it (without the input and output layers), as exemplified by Fig. 1. This is formalized below.

**Definition 4.2.** Consider a neural network \( f : (\mathbb{R}^d)^k \to \mathbb{R} \) with input embedding matrices \( U^1, \ldots, U^k \in \mathbb{R}^{n \times d} \) (not necessarily distinct) and readout matrix \( V \in \mathbb{R}^n \), so that \( f(x^1, \ldots, x^k) = V^T \Phi(U^1 x^1, \ldots, U^k x^k; \Theta) \) for some function \( \Phi(x^1, \ldots, x^k; \Theta) \) with parameters \( \Theta \). We say a NetTOR{T} program represents \( f \) if it computes \( \Phi \) (under some correspondence of \( \mathcal{V} \cup \mathcal{W} \) to \( \{x^1, \ldots, x^k\} \cup \Theta \)).\(^{14}\)

For example, the programs in Fig. 1 resp. represent a 3-hidden-layer MLP and an RNN running for 3 steps. Note that the initial vectors correspond to a combination of input embeddings (e.g. \( W^3 \xi \)) and vector parameters (e.g. biases) and the matrices correspond to matrix parameters (e.g. weights).

\(^{13}\)One can see this easily by modifying our calculations above.

\(^{14}\)We only consider \( f \) with scalar output for simplicity but generalization to multi-dimensional output is straightforward.
Intuition for a Program in the Large n Limit. Typically, the vectors (resp. matrices) in a program will be sampled iid like \( \mathcal{N}(0, 1) \) (resp. \( \mathcal{N}(0, 1/n) \)), corresponding to the “standard” initialization of neural networks.\(^{16}\) In such cases, when \( n \to \infty \), a program behaves as follows, in a gist:

IID Coordinates Any vector \( x \in \mathbb{R}^n \) in the program has roughly iid coordinates. We write \( Z^x \) for the random variable encoding this coordinate distribution. This \( Z^x \) may be correlated with \( Z^y \) for other vector \( y \) in the program, such that, for example, \( \lim_{n \to \infty} x^T y/n = \mathbb{E} Z^x Z^y \).

Nonlin \( Z^{\psi(x^1, \ldots, x^k)} = \psi(Z^{x^1}, \ldots, Z^{x^k}) \).

MatMul, without \( (W, W^\top) \)-Interaction Consider a matrix \( W \in \mathbb{R}^{n \times n} \) in the program and any set of \( \mathbb{R}^n \) vectors \( X \) not dependent on vectors of the form \( W^\top \cdot \). Then the set of random variables \( \{Z^{W^x} : x \in X\} \) are jointly Gaussian with mean zero and covariance \( \text{Cov}(Z^{W^x}, Z^{W^y}) = \mathbb{E} Z^x Z^y \) for any \( x, \tilde{x} \in X \). If \( W \neq W \) is another matrix in the program and \( Y \) is a set of such vectors w.r.t. \( W \), then the set \( \{Z^{W^x} : x \in X\} \) is independent from \( \{Z^{W^y} : y \in Y\} \).

MatMul, with \( (W, W^\top) \)-Interaction For general \( x, Z^{W^x} \) decomposes into a sum of a Gaussian part, identical to \( Z^{W^x} \) in the above case, and a correction term. This decomposition is a generalization of Eq. (17).

See Theorem B.4 for formal details.

NETSOR\(^{\top+} \) Programs (Yang, 2019a; 2020a) showed that NETSOR\(^{\top} \) suffices to express the forward and backward passes of most architectures such as ResNet (with Batchnorm), but Transformer and other standard architectures require adding to NETSOR\(^{\top} \) a new “averaging” instruction\(^{16} \) that returns the “empirical average” \( \frac{1}{n} \sum_{\alpha=1}^n x_\alpha \) of a vector \( x \in \mathbb{R}^n \). In the \( n \to \infty \) limit, this scalar converges to \( \mathbb{E} Z^x \) as would be expected from the intuitions above. This extension of NETSOR\(^{\top} \) (called NETSOR\(^{\top+} \)) also allows us to express the network output and loss derivative (e.g. in contrast to Fig. 1), which will be a technical requirement for unrolling the entirety of SGD training inside a single program, a key step in the proof of our main result. See discussion of proof formalization in Section 5. We can say a NETSOR\(^{\top+} \) program represents a network \( f \) if it computes the body of \( f \).

5. Universality of Kernel Dynamics

(Yang, 2019a; 2020a) showed that any neural network of standard architecture is represented by a NETSOR\(^{\top+} \) program. Moreover,

**Theorem 5.1** (Yang (2020a)). For a neural network as in Setup 5.2 below, its Neural Tangent Kernel at initialization has a well-defined infinite-width limit \( \bar{K} \).

**Setup 5.2** (Representable NN in NTK Parametrization). Suppose a neural network \( f \) is represented by a NETSOR\(^{\top+} \) program (in the sense of Definition 4.2) whose NONLIN all have polynomially bounded derivatives.\(^{17} \) Adopt the NTK parametrization: for every matrix parameter \( W \in \mathbb{R}^{n \times n} \) of \( f \), we factor \( W = \frac{1}{\sqrt{n}} w \) where \( w \) is the trainable parameter; likewise, for each input layer matrix \( U^i \in \mathbb{R}^{n \times d} \), we factor \( U^i = \frac{1}{\sqrt{d}} u^i \), and likewise the output matrix \( V = \frac{1}{\sqrt{d}} v \), such that \( u^i, v \) are trainable. Finally, we randomly initialize all trainable parameters iid as \( \mathcal{N}(0, 1) \).

Our main result is to show that the SGD training of such a neural network described in Setup 5.2 reduces to kernel gradient descent with kernel \( \bar{K} \) in the infinite-width limit.

**Theorem 5.3** (NTKTrain is Architecturally Universal). Consider training a network \( f \) described in Setup 5.2 via SGD with batch-size 1 and (WLOG) learning rate 1. Let \( \xi_t \) be the input and \( L_t : \mathbb{R} \to \mathbb{R} \) be the loss function (absorbing the label) at time \( t \). Suppose \( L_t \) is continuous for all \( t \). Then, for any \( \xi \) and \( t \), \( f_t(\xi) \) converges almost surely to a random variable \( \hat{f}_t(\xi) \) as \( \text{width} \to \infty \), such that

\[
\hat{f}_{t+1}(\xi) - \hat{f}_t(\xi) = -\bar{K}(\xi, \xi_t) L'_t(\hat{f}_t(\xi_t))
\]

where \( \bar{K} \) is the infinite-width NTK (at initialization) of the neural network.

The full proof of Theorem 5.3 is given Appendix D.

**Extension** We briefly mention several ways our result can be easily extended. 0) Different batch sizes, learning rate schedules, and nonscalar outputs. 1) Variants of NTK parametrization. We can deal with any parametrization that scales the same way as NTK parametrization, e.g. weights are sampled like \( \mathcal{N}(0, \sigma^2) \) for any \( \sigma \), with the multipliers \( \gamma/\text{fanin} \) for any \( \gamma \). 2) Variable width. In real networks, the width of different layers can often be different (e.g. in ResNet). Our result can be extended to the case where the widths tend to infinity at a fixed ratio, using the variable-width version of Tensor Programs (Yang, 2020b). 3) Unsupervised and other learning settings can be covered because their training and testing computation can be written into Tensor Programs. 4) Weight decay, momentum, and other optimizer tricks can be covered as well as they can be straightforwardly written into Tensor Programs, but in general the kernel will change from step to step in contrast to Theorem 5.3.
5.1. Proof Sketch of Special Case

To convey the main idea, we give a proof sketch of a simplified problem: we assume 1) the input, output layers and biases are not trained (the network has only $\mathbb{R}^{n \times n}$ matrices as trainable parameters); 2) the forward pass does not contain both a weight matrix $W$ and its transpose $W^T$ (but a single matrix $W$ can still be used multiple times without being transposed); 3) input space is $\mathbb{R}^n$ (with $k = 1$), and $f = V^T x \in \mathbb{R}$; 4) the output vector $x$ is a G-var; 5) the network is represented by a NETSOR $^\top$ (instead of NETSOR $^\top$) program. In the appendix, we prove the general case with these simplifications lifted.

It turns out, every NETSOR $^\top$ can be simplified into a standard form of sorts, which greatly facilitates our proof.

**Definition 5.4.** In a NETSOR $^\top$ program, a G-var is an initial vector or a vector created by MATMUL, while an X-var is a vector created by NONLIN. We define a reduced NETSOR $^\top$ program as a program in which only G-vars are allowed as inputs to a NONLIN, while only an X-var is allowed as input to a MATMUL.

Observe that any NETSOR $^\top$ program may be trivially expressed as a reduced NETSOR $^\top$ program by: 1) collapsing chains of non-linearities which appear consecutively, and 2) insert a NONLIN operation with $\psi(x) = x$ in between consecutive G-vars. Hence, we may safely assume that $f$ is representable by a reduced NETSOR $^\top$ program.

**Key Idea: Paths.** The examples of Sections 3.1 and 3.2 exposed several insights, such as the iid-coordinates intuition, important for proving Theorem 5.3. Now we discuss the one remaining key idea for scaling up to general architectures:

**Definition 5.5 (Paths).** In a NETSOR $^\top$ program, a path $p$ starts with an X-var and ends with a G-var, alternating between X- and G-vars along the path. We write $p^0$ for the starting X-var, $p^i$ for the following G-var, and so on, as well as $p^{-1}$ for the ending G-var (see Fig. 2 for a graphical illustration). For odd $i$, let $W^{p_i}$ denote the defining matrix of G-var $p_i$. For two equal length paths $p, q$, we write $p \cong q$ (path $p$ is isomorphic to path $q$) if for all odd $i$, $W^{p_i}$ is the same matrix as $W^{q_i}$. In other words, we say path $p$ is isomorphic to path $q$ if their sequences of MATMUL matrices are identical, but the NONLIN don’t have to be, see Fig. 3 for a graphical illustration). Let $|p|$ denote the number of vectors in $p$ (this is always an even number).

The collection of paths $p$ starting with an X-var $p^0 = x$ and

$$\text{end with a G-var } h \text{ describes all possible pathways of backpropagating an error signal } dh \text{ at } h \text{ to an error signal } dx \text{ at } x. \text{ Simultaneously, it also describes all possible pathways of forward propagating a change in } x \text{ to a change in } h. \text{ }

**Decomposing the Change in } f \text{ to a Sum over Paths** Because the gradient $\nabla W f$ of a weight $W \in \mathbb{R}^{n \times n}$ is the sum of outer products $\sum h, x = W x dh \otimes x$, summing over all G-vars $h$ and X-vars $x$ in the program with $h = W x$ (where $dh$ denotes $\nabla h, f$), we also have

$$\nabla W f = \sum_{h, x; h = W x} \sum_p J^p \otimes x.$$ \hspace{1cm} (23)

where

$$(J^p)^\top = \frac{\partial f}{\partial p^{−1}} \times \frac{\partial p^{−2}}{\partial p^{−3}} \times \ldots \times \frac{\partial p^2}{\partial h}.$$ \hspace{1cm} (24)

i.e., $J^p$ denotes the error signal at $h$ from backpropagation through path $p$, and $p$ ranges over all paths starting with $p^0 = x, p^i = h$ and ending with the output node of the underlying program. Recall $W$ factors as $\frac{1}{\sqrt{n}}$ where $w$ is the trainable parameter, not $W$. By the discussion above, updating $w$ with $\nabla_w f = \frac{1}{\sqrt{n}} \nabla W f$ causes $f$ to change by

$$\left \langle \frac{1}{\sqrt{n}} \nabla W f, \frac{1}{\sqrt{n}} \nabla W f \right \rangle \hspace{1cm} (25)$$

When every parameter $w$ is randomized iid as $\mathcal{N}(0, 1)$, it turns out that $\langle J^p, J_p \rangle$ will go to 0 as $n \to \infty$ unless $p \cong \bar{p}$ (Definition 5.5). If one think of $J^p$ as a product of random Gaussian matrices (interleaved with other matrices), then this is akin to the fact that, for a mixed moment $M \overset{\text{def}}{=} \mathbb{E} \prod_{i=1}^{k} Z_{\gamma(i), \gamma} : [r] \to [k]$ of standard iid
While the core ideas discussed above are intuitive, mak-
we have
The key insight is similar to Eq. (4) in the 1-hidden-layer
grams framework. The mechanics of the proof then goes
as follows: 1) First we unroll SGD of \( f \) into a NETSOR \( T \)
program. \(^{22}\) This is similar to the equations in Sections 3.1
and 3.2; the key here is to express \( \delta x_{t+1} = \sqrt{n}(x_{t+1} - x_t) \)
as a vector in the program, for any (pre-)activation \( x \). 2) We
apply the NETSOR \( T \) Master Theorem (Yang, 2020b) to
this program. This yields the coordinate distribution of each
vector. The core insights here are demonstrated by the calcula-
tion with the \( Z \) random variables in Sections 3.1 and 3.2.
3) Finally, we need to show that (the rigorous version of)
Eq. (26) indeed recovers the NTK and agrees with Eq. (22).
This is done via an inductive (symbolic) computation, and
the path concept in this section plays a key role here.

6. Related Works

The connection between kernel methods and neural net-
works has had a long history before its recent resurgence.
The Gaussian Process (NNGP) view of wide neural net-
works, which characterizes the behaviour of training only
the last layer of a wide neural network, has been studied in
(Daniely et al., 2016; Hazan & Jaakkola, 2015; Roux & Ben-
gio, 2007; Lee et al., 2018; Matthews et al., 2018; Hinton
& Neal, 1995; Novak et al., 2019). Since the original NTK
paper (Jacot et al., 2018), many works have informally de-
"rived the infinite-width NTK for various architectures such as
CNNs (Arora et al., 2019), RNN (Alemohammad et al.,
2020), attention (Hron et al., 2020), ensembles (Littwin
et al., 2020b) and graph neural networks (Du et al., 2019),
but none of them formally proved \( \text{NTK}\text{INIT} \) or \( \text{NTK}\text{TRAIN} \)
for those architectures. Finite width corrections to the NTK
were derived for fully connected networks in (Hanin & Nica,
2019; Littwin et al., 2020a). The validity of the NTK theory
was empirically studied in (Lee et al., 2019) for a variety of
architectures.

The Tensor Program framework (Yang, 2019a; 2020a;b)
was introduced in an attempt to unify and generalize the
NNGP/NTK theory to a broad range of architectures, elimi-
nating the need to re-develop the theory for each new ar-
chitecture. For example, (Yang, 2019a) proved the architec-
tural universality of NNGP correspondence, while (Yang,
2020a) proved that of \( \text{NTK}\text{INIT} \). On the other hand, (Yang,
2020b) developed the most general machinery for Tensor
Programs and as a corollary constructed a comprehensive
theory of nonlinear random matrix theory, that, for exam-
ple, can calculate the singular value distribution of a wide
neural network of any architecture. Our proofs depend on
the machinery of (Yang, 2020b) crucially, as discussed in
Section 5.

\(^{22}\) We note that this formalization crucially relies on NETSOR \( T \)
and its Master Theorem from (Yang, 2020b) because the SGD
unrolling cannot be done in NETSOR \( T \). The reason is that we need
to express the output and loss derivatives of the network, which
are scalars (or at least finite dimensional), and that cannot be done in
a NETSOR \( T \) program. Furthermore, the Master Theorem from
(Yang, 2020a) only pertains to a specific type of programs that look
like the first backpropagation after initialization. Thus, it cannot
deal with the complete unrolling of SGD as we do here, which
requires the more advanced Master Theorem from (Yang, 2020b).

Putting It All Together and Proof Formalization

While the core ideas discussed above are intuitive, mak-
ing them rigorous at face value would be quite challenging.
Instead we use the machinery offered by the Tensor Pro-
grams framework. The mechanics of the proof then goes
as follows: 1) First we unroll SGD of \( f \) into a NETSOR \( T \).

Figure 3: Paths Isomorphism. A graphical illustration of
path isomorphism for paths \( p, q \) with \( |p| = |q| = 2 \) in an
MLP and RNN. In the MLP example, \( p \) is not isomorphic to
\( q \) because the weights \( W^{-1}, W^2 \) defining the vectors \( p^1, q^1 \)
are not identical. For the RNN, \( p \) is isomorphic to path \( q \)
because \( p^1 \) and \( q^1 \) are defined with the same weight \( W \).

Gaussians \( Z_1, \ldots, Z_k \), \( M \) is nonzero iff every \( Z_i \) appears
an even number of times in the product. This means we can
replace the 4 nested sums in Eq. (25) with the single sum
\( \sum_{p \neq p} \) and rewrite \( x = p^0, \bar{x} = \bar{p}^0 \).

We have suppressed dependence on input in Eq. (25). Being
more explicit about it and performing updates on all weights, we have

\[
\begin{align*}
    f_{t+1}(\xi) - f_t(\xi) & \approx -\mathcal{L}'(f_t(\xi)) \sum_{p \neq p} \langle J^p(\xi), J^p(\xi) \rangle \langle p^0(\xi), \bar{p}^0(\xi) \rangle. 
\end{align*}
\]  

after taking a gradient step on input \( \xi_t \) at initialization \( t = 0 \).
(Here \( p^0(\xi) \) denotes the vector \( p^0 \) as a function of \( \xi \) at
initialization). However, Eq. (25) holds for general \( t \) as well:
The key insight is similar to Eq. (4) in the 1-hidden-layer
example, that vectors \( p^0(\xi), J^p(\xi) \), etc change vanishingly
from their initial values as \( n \to \infty \), after any number of
SGD steps. Because our arguments above only depend on
inner products between vectors, this means that the error
in Eq. (26) for \( t > 0 \) vanishes as \( n \to \infty \). Finally, at
least heuristically, it is straightforward to show the RHS of
Eq. (26) is the NTK via a series of calculations exemplified
by those in Sections 3.1 and 3.2, to get Eq. (22).
7. Conclusion

New theories of deep learning almost always start with MLPs, rightly so as they are the simplest case and can often reveal the key insights more clearly. Of course, as deep learning itself is an applied field, one should always ask whether insights on MLPs extend to more general architectures, i.e. whether there is an *architecturally universal extension* of a proposed theory of MLPs. This is not always easy to answer.

In this paper, we showed that the NTK theory is architecturally universal, but more importantly, we showed that the Tensor Programs technique is a very powerful tool for answering the above question as a matter of routine. Looking forward, we hope to apply it to generate more novel and general insights.
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Architectural Universality of Neural Tangent Kernel Training Dynamics

Appendix organization The appendix is organized as follows:
In Appendix A we expand upon the examples given in Section 3, while adding some additional details.
In Appendix B we introduce the formal version of the NETSOR, NETSOR\(+\) programs.
In Appendix C we introduce the graphical notation of NETSOR\(+\) and demonstrate other examples of architectures or computations expressible in Tensor Programs.
In Appendix D we prove our main result.

Notations For the readers convenience we restate the notations described in Section 2, along with some additional ones which will be used throughout the appendix. We will consider SGD with batch size 1 and learning rate of 1 (WLOG). We use \( \xi \) to denote the input and \( L_t \) to denote the loss function (absorbing the label) at step \( t \). More generally, subscript \( t \) on any symbol means time \( t \). However, for brevity, we abuse notation and shorthand \( f_t \) for \( f_t(\xi_t) \), and, for any (pre-)activation \( x, x_t \) for \( x_t(\xi_t) \). We will also write \( \chi_t \) for the loss derivative \( L'_t(f_t) \). For any vector \( x(\xi) \) we define \( \delta x_{t+1}(\xi) \equiv \sqrt{n}(x_{t+1}(\xi) - x_t(\xi)) \) and \( d x(\xi) \equiv \sqrt{n}\frac{\partial f(\xi)}{\partial x(\xi)} \). We will track the evolution of \( f \) on an arbitrary input \( \tilde{x} \).

Similar to above, we shorthand \( \tilde{x_t}, \tilde{f}_t \) for \( x_t(\tilde{\xi}), f_t(\tilde{x}) \). In general, omitting the time index \( t \) for any time dependent quantity implies its value at initialization. (i.e \( x(\xi) = x_0(\xi), f(\xi) = f_0(\xi) \)). Finally, we use \( \triangleq \) to imply equality of symbols (i.e \( W^1 \triangleq W^2 \) iff \( W^1, W^2 \) represent the same variable, as opposed to equality in value).

A. Additional Examples

In this section we flesh out the examples given in Section 3 of the main text with the purpose of adding additional clarity, while maintaining the intuitive arguments as presented in each example to perform these calculations. The rigorous justification for these calculations will be given in the following section with the formal introduction of the Tensor Program framework.

Recall that our objective is to derive Claim 3.1 by tracking the coordinate distribution of each (pre-)activations vector \( x(\xi), d x(\xi) \equiv \sqrt{n}\frac{\partial f(\xi)}{\partial x(\xi)}, \delta x(\xi) \equiv \sqrt{n}(x_{t+1}(\xi) - x_t(\xi)) \).

**Claim 3.1.** In the large width limit, \( \tilde{f}_t = f_t(\tilde{\xi}) \) changes by

\[
\lim_{n \to \infty} \tilde{f}_{t+1} - \tilde{f}_t = -\chi_t \tilde{K}(\tilde{\xi}, \xi_t)
\]

at step \( t \), where \( \tilde{K} \) is the limiting NTK of the architecture and \( \chi_t = L'_t(\lim_n f_t) \) is the loss derivative.

In our calculations we will rely on the following rules relating to the coordinates of any \( \mathbb{R}^n \) (pre-)activation vector \( x(\xi) \) in the large width regime, which we will later formalize:

- \( x_{t+1}(\xi) - x_t(\xi) \) has \( \Theta(\frac{1}{\sqrt{n}}) \) coordinates.
- \( \delta x_{t+1}(\xi) \) has \( \Theta(1) \) coordinates.
- \( x_t(\xi) = x(\xi) + o(1) \). Consequently \( Z^{x_t(\xi)} = Z^x(\xi) \).
- If \( x(\xi) = \phi(y(\xi)) \) for some vector \( y(\xi) \in \mathbb{R}^n \), then by Taylor approximation \( \delta x_{t+1}(\xi) = \sqrt{n}(\phi(y_t(\xi)) + \frac{\delta y_{t+1}(\xi)}{\sqrt{n}} - \phi(y_t(\xi))) \approx \phi'(y_t(\xi)) \odot \delta y_{t+1}(\xi) \). Consequently \( Z^{\delta x_{t+1}(\xi)} = \phi'(Z^y(\xi))Z^{\delta y_{t+1}(\xi)} \).

**Remark A.1.** We write \( Z^x \) to denote the limit coordinate distribution of \( x \in \mathbb{R}^n \) conditioned on the output function \( f \) at initialization. Consequently we write \( \mathbb{E} X^Z \) to express a conditional expectation given the output function \( f \). See Appendix B for the formal statement.

### A.1. 1 hidden layer

Recall our model is of the form:

\[
f = V^\top x, \quad x = \phi(h), \quad h = U \xi\]

where \( \xi \in \mathbb{R}^d, U = \frac{u}{\sqrt{d}} \in \mathbb{R}^{n \times d}, V = \frac{v}{\sqrt{n}} \in \mathbb{R}^{n \times 1} \), for trainable parameter tensor \( u \), initialized iid from \( \mathcal{N}(0, 1) \), and \( d = 1 \).

\( ^{23} \)It might help to think of \( \tilde{\xi} \) as some test sample, but it can also fall in the training set.
Deriving The NTK  The infinite width NTK of this architecture is given by:

\[
\mathcal{K}(\xi, \tilde{\xi}) = \langle \nabla_u f(\xi), \nabla_u f(\tilde{\xi}) \rangle = \xi^\top \mathbb{E} \left[ \frac{\partial f(\xi)}{\partial h(\xi)} \right] \tilde{\xi}
\]

(27)

\[
dh(\xi) \overset{\text{def}}{=} \sqrt{n} \frac{\partial f(\xi)}{\partial h(\xi)} = \phi'(h(\xi)) \odot v.
\]

(28)

Therefore, by LLN it follows:\(^{24}\)

\[
\hat{\mathcal{K}}(\xi, \tilde{\xi}) = \xi^\top \lim_{n \to \infty} \frac{1}{\sqrt{n}} \mathbb{E} \left[ \frac{\partial f(\xi)}{\partial h(\xi)} \right] \tilde{\xi} = \xi^\top \mathbb{E} \phi'(Z^h(\xi)) \phi'(Z^h(\xi)).
\]

(29)

Getting Claim 3.1  To show that Claim 3.1 holds with the kernel in Eq. (29), we track the coordinate distribution \(Z^\delta_{t+1}\) at each step of SGD. At step \(t\), the update to the weights \(u_{t+1} - u_t\) is given by the gradient of the loss with respect to \(u_t\):

\[
u_{t+1} - u_t = -\chi_t \frac{dh_t}{\sqrt{n}}, \quad dh_t = \phi'(h_t) \odot v
\]

(30)

Recall that \(\delta h_{t+1} = \sqrt{n}(h_{t+1} - h_t) = \sqrt{n}(u_{t+1} \bar{\xi} - u_t \bar{\xi})\) and \(\delta \bar{x}_{t+1} = \sqrt{n}(\bar{x}_{t+1} - \bar{x}_t).\) It therefore follows:

\[
\delta h_{t+1} = -\chi_t \xi_t^\top \xi \phi'(h_t) \odot v, \quad \delta \bar{x}_{t+1} = \sqrt{n}(\phi(h_t + \delta h_{t+1}) - \phi(h_t)).
\]

(31)

Since \(h_t = \Theta(1)\) and \(\delta h_{t+1} = \Theta(1)\), for large \(n\) we may Taylor expand \(\phi\) to first order around \(\bar{h}_t\):

\[
\delta \bar{x}_{t+1} \approx \sqrt{n}(\phi(h_t) + \frac{1}{\sqrt{n}} \phi'(h_t) \odot \delta h_{t+1} - \phi(h_t))
\]

(32)

\[
= \phi'(\bar{h}_t) \odot \delta \bar{x}_{t+1}
\]

(33)

\[
= -\chi_t \xi_t^\top \xi \phi'(h_t) \odot v.
\]

(34)

Again since \(\delta h_t(\xi) = \Theta(1)\), it follows that \(h_t(\xi) = h(\xi) + \sum_{s=1}^{t} \frac{\delta h_s(\xi)}{\sqrt{n}} = h(\xi) + o(1)\). Hence, in the infinite width limit the coordinate distribution of \(h_t(\xi)\) is identical to the coordinate distribution of \(h(\xi)\) (i.e \(Z^h(\xi) = Z^h(\xi)\)). Using Eq. (34), the coordinate distribution of \(\delta \bar{x}_{t+1}\) is given by:

\[
Z^\delta \bar{x}_{t+1} = -\chi_t \xi_t^\top \xi \phi'(Z^h) \phi'(Z^h) Z^v.
\]

(35)

In the large width limit, the change in the output is simply given by \(\tilde{f}_{t+1} - \tilde{f}_t = \frac{v^\top \delta \bar{x}_{t+1}}{n} = \mathbb{E} Z^\delta \bar{x}_{t+1} Z^v\). Using Eq. (35) and the independence of \(Z^v\) from the other random variables,\(^ {25}\)

\[
\mathbb{E} Z^\delta \bar{x}_{t+1} Z^v = -\mathbb{E} \chi_t \xi_t^\top \xi \phi'(Z^h) \phi'(Z^h) Z^v
\]

(36)

\[
= -\chi_t \xi_t^\top \xi \phi'(Z^h) \phi'(Z^h)
\]

(37)

\[
= -\chi_t \hat{\mathcal{K}}(\xi_t, \tilde{\xi})).
\]

(38)

A.2. 2 hidden layers

Recall our model is of the form:

\[
f = V^\top x, \quad x = \phi(h), \quad h = Wz
\]

\[
z = \phi(g), \quad g = U \xi
\]

where \(U = \frac{1}{\sqrt{n}} \in \mathbb{R}^{n \times d}\), \(W = \frac{1}{\sqrt{n}} \in \mathbb{R}^{n \times n}\), \(V = \frac{1}{\sqrt{n}} \in \mathbb{R}^{n \times 1}\), for trainable parameters \(u, w, \) initialized iid from a normal distribution. As before we assume the last layer is not trained, and \(d = 1\).

\(^{24}\)While in Remark A.1, we said \(\mathbb{E}\) denotes expectation conditioned on \(\lim f_0\), the NTK here does not actually depend on \(\lim f_0\).  

\(^{25}\)Again, as in Footnote 10, the expectations in Appendices A.1 and A.2 should more rigorously be interpreted as expectation conditional on the function values of \(\lim f_0\).
Deriving The NTK

The infinite width NTK is given by:

\[ K(\xi, \tilde{\xi}) = \langle \nabla_u f(\xi), \nabla_u f(\tilde{\xi}) \rangle + \langle \nabla_w f(\xi), \nabla_w f(\tilde{\xi}) \rangle = \xi^T \xi^T \delta g(\xi)^T \delta g(\tilde{\xi}) + \frac{z(\xi)^T z(\tilde{\xi})}{n} dh(\xi)^T dh(\tilde{\xi}) \]

(39)

(40)

\[ dh(\xi) \triangleq \sqrt{n} \frac{\partial f(\xi)}{\partial h(\xi)} = \phi'(h(\xi)) \odot v \]

(41)

\[ dg(\xi) \triangleq \sqrt{n} \frac{\partial f(\xi)}{\partial g(\xi)} = \phi'(g(\xi)) \odot (W^T dh(\xi)). \]

(42)

Naively using LLN on Eq. (39) (and \( Z^n \) being independent from everything else) should result in:

\[ K(\xi, \tilde{\xi}) = \xi^T \xi \mathbb{E} [Z^d(\xi) Z^d(\tilde{\xi})] + \mathbb{E} [Z^z(\xi) Z^z(\tilde{\xi})] \mathbb{E} \phi'(Z^h(\xi)) \phi'(Z^h(\tilde{\xi})). \]

(43)

Evaluating the term \( \mathbb{E} [Z^d(\xi) Z^d(\tilde{\xi})] \) however presents a challenge since \( dh(\xi) \) depends on both \( W \) and \( W^T \). As it turns out, at initialization we may naively assume that \( W^T, W \) are independent (formally known in the literature as gradient independence assumption, or GIA) \(^\text{26}\), we arrive using simple LLN arguments to:

\[ \mathbb{E} [Z^d(\xi) Z^d(\tilde{\xi})] = \mathbb{E}[\phi'(Z^g(\xi)) \phi'(Z^g(\tilde{\xi}))] \mathbb{E}[\phi'(Z^h(\xi)) \phi'(Z^h(\tilde{\xi}))]. \]

(44)

Plugging Eq. (44) into Eq. (43) we arrive at the correct expression for the infinite width NTK.

Getting Claim 3.1

To show that Claim 3.1 holds at any step \( t \) (where we may not assume that GIA holds), we track the distributions of the vectors \( g(\xi), z(\xi), h(\xi), x(\xi) \) throughout training.

At any step \( t \) the weights are updated according to:

\[ u_{t+1} - u_t = -\chi_t \frac{dg u_t^T}{\sqrt{n}}, \quad w_{t+1} - w_t = -\chi_t \frac{dh u_t^T}{n}. \]

(45)

The update \( \delta g_{t+1} \triangleq \sqrt{n}(\tilde{g}_{t+1} - \tilde{g}_t), \delta z_{t+1} \triangleq \sqrt{n}(\tilde{z}_{t+1} - \tilde{z}_t) \) are given by:

\[ \delta \tilde{g}_{t+1} = -\chi_t d g_{t+1}^T \tilde{\xi}, \quad \delta \tilde{z}_{t+1} = \sqrt{n}(\phi(\tilde{g}_t + \delta \tilde{g}_{t+1}) - \phi(\tilde{g}_t)). \]

(46)

As before, with large \( n \) we have that \( \bullet_{t+1}(\xi) - \bullet_t(\xi) \sim \Theta(\frac{1}{\sqrt{n}}) \) and \( \delta \bullet_{t+1}(\xi) \sim \Theta(1) \) coordinates for \( \bullet \) replaced by \( \{g, z, h, x\} \). And so after Taylor expanding \( \phi(\tilde{g}_t + \delta \tilde{g}_{t+1}) \) around \( \tilde{g}_t \):

\[ \delta \tilde{z}_{t+1} \approx \phi'(\tilde{g}_t) \odot \delta \tilde{g}_{t+1}. \]

(47)

In a similar fashion, using Eqs. (41) and (46) the updates \( \delta \tilde{z}_{t+1}, \delta \tilde{x}_{t+1}, \delta \tilde{z}_{t+1} \) take the form:

\[ \delta \tilde{z}_{t+1} \approx \phi'(g_t) \odot \delta g_t + \frac{1}{\sqrt{n}} \sum_{s=0}^{t} \chi_s z_s^T \delta \tilde{z}_{t+1} \phi'(h_s) \odot v \]

(48)

\[ \delta \tilde{h}_{t+1} = \sqrt{n}(W_{t+1} - W_t) \tilde{z}_t \]

(49)

\[ \delta \tilde{x}_{t+1} \approx \phi'(h_t) \odot \delta \tilde{h}_{t+1}. \]

(50)

where we used Eq. (45) and

\[ \delta \tilde{h}_{t+1} = W_{t+1} \delta \tilde{z}_{t+1} + \sqrt{n}(W_{t+1} - W_t) \tilde{z}_t \]

(51)

\[ W_{t+1} \delta \tilde{z}_{t+1} + \sum_{s=0}^{t} (W_{s+1} - W_s) \delta \tilde{z}_{t+1} + \sqrt{n}(W_{t+1} - W_t) \tilde{z}_t \]

(52)

\(^\text{26}\)For a rigorous justification of the GIA assumption see (Yang, 2020a)
to get Eq. (49). Based on Eqs. (41) and (48) to (50), the corresponding coordinate distributions take the form:

\[ Z_{dhi}^{dh} = \phi'(Z_{hi}^{h})Z^{v} \]  
(53)

\[ Z_{d\xi+1} = -\tilde{\chi}_{t}\xi_{t}^{T}\tilde{\xi}\phi'(Z_{g}^{h})\phi'(Z_{\bar{g}}^{h})Z^{W}Z_{dhi}^{dh} \]  
(54)

\[ Z_{d\xi+1} = Z^{W\tilde{\xi}+1} - \tilde{\chi}_{t}E[Z_{\bar{v}}^{Z_{\bar{v}}}\phi'(Z_{h}^{h})Z^{v}] \]  

As before, the functional update is given by

\[ \lim_{n \to \infty} Z_{\xi+1} = \Phi(Z_{\xi}^{\xi}) - E[Z_{\xi}^{\xi}] \Rightarrow \Phi(Z_{\xi}^{\xi}) = Z_{\xi}^{\xi}. \]  

To compute the second term of the RHS of Eq. (57), we use Claim 3.2, reproduced below.

**Claim 3.2.** Based on the above discussion and some easy calculations, \( \delta_{\xi+1} \) can be written as \( \Phi(W^{T}dh) \) for some \( \Phi : R \to R \) applied coordinatewise (which will depend on other vectors not of the form \( W^{T} \)). Then it turns out

\[ Z^{W\delta_{\xi+1}} = G + Z^{dh}E[\delta_{\xi+1}] \]  
(17)

where \( G \) is some Gaussian variable independent from \( Z^{v} \), and \( \frac{\partial Z^{W\delta_{\xi+1}}}{\partial Z^{W^{T}dh}} \equiv \Phi'(Z^{W^{T}dh}) \).

Applying Claim 3.2 to get the expression for \( Z^{W\delta_{\xi+1}} \):

\[ Z^{W\delta_{\xi+1}} = G + Z^{dh}E[\delta_{\xi+1}] \]  
(58)

\[ = G - \phi'(Z_{h}^{h})E[\tilde{\chi}_{t}\xi_{t}^{T}\tilde{\xi}\phi'(Z_{g}^{h})\phi'(Z_{\bar{g}}^{h})] \]  

As before, for \( h \in \{ g, z, h, x \} \) it holds that \( h_{t}(\xi) = h(\xi) + \sum_{s=1}^{t}\frac{\delta h_{r}(\xi)}{\sqrt{n}} = h(\xi) + o(1) \), and \( Z^{h_{r}(\xi)} = Z^{h(\xi)} \). Plugging Eq. (58) into Eq. (57) yields Claim 3.1.

**B. Tensor Programs: the Formal Version**

We briefly review the formal definition of Tensor Programs below, but readers needing more explanation and intuition should see (Yang, 2020b). We will directly describe NETSOR\( ^{T} \) programs, which generalizes NETSOR \( ^{T} \).

**Definition B.1.** A NETSOR\( ^{T} \) program is a sequence of \( R^{n} \)-vectors and \( R \)-scalars inductively generated via one of the following ways from an initial set \( C \) of random scalars, \( \mathcal{V} \) of random \( R^{n} \) vectors, and a set \( \mathcal{W} \) of random \( R^{n \times n} \) matrices (which will be sampled with iid Gaussian entries in Setup B.2)

\[ \text{MATMUL} \text{ same as MATMUL in Definition 4.1.} \]

**NONLIN** Given \( \phi : R^{k} \times R^{l} \to R \), previous scalars \( \theta_{1}, \ldots, \theta_{l} \in R \) and vectors \( x^{1}, \ldots, x^{k} \in R^{n} \), we can generate a new vector

\[ \psi(x^{1}, \ldots, x^{k}; \theta_{1}, \ldots, \theta_{l}) \in R^{n} \]  
(60)

where \( \psi(-; \theta_{1}, \ldots, \theta_{l}) \) applies coordinatewise to each “\( \alpha \)-slice” \( (x_{\alpha}^{1}, \ldots, x_{\alpha}^{k}) \).

**MOMENT** Given same setup as above, we can also generate a new scalar

\[ \frac{1}{n} \sum_{\alpha=1}^{n} \psi(x_{\alpha}^{1}, \ldots, x_{\alpha}^{k}; \theta_{1}, \ldots, \theta_{l}) \in R. \]  
(61)

A NETSOR\( ^{T} \) program is just a NETSOR\( ^{T} \) program without scalars, without the usage of MOMENT, and without parameters \( \theta_{1}, \ldots, \theta_{l} \) in NONLIN\( ^{+} \).

We will typically randomly sample the initial matrices, vectors, and scalars of the program as follows.
**Setup B.2.** 1) For each initial $W \in \mathcal{W}$, we sample iid $W_{\alpha \beta} \sim \mathcal{N}(0, \sigma_W^2/n)$ for some variance $\sigma_W^2$ associated to $W$, independent of other $W' \in \mathcal{W}$; 2) for some multivariate Gaussian $Z^V = \{Z^h : h \in \mathcal{V}\} \in \mathbb{R}^V$, we sample the initial set of vectors $\mathcal{V}$ like $\{h_\alpha : h \in \mathcal{V}\} \sim Z^V$ iid for each $\alpha \in [n]$. 3) For each initial scalar $\theta \in \mathcal{C}$, we require $\theta \overset{\text{a.s.}}{\longrightarrow} \hat{\theta}$ for some deterministic $\hat{\theta} \in \mathbb{R}$.

The following constructs a random variable $\hat{Z}^h$ for every vector $h$ and a deterministic scalar $\hat{\theta}$ for every scalar $\theta$ in the program. The interpretation is that $h$ will have iid coordinates distributed like $\hat{Z}^h$, and $\theta$ will converge to $\hat{\theta}$ as $n \to \infty$.

**Definition B.3 ($\hat{Z}^h$ and $\hat{\theta}$).** Given a NETSOR$\uparrow$ program, we recursively define $\hat{Z}^h$ for each vector $h$ and $\hat{\theta}$ for each scalar $\theta$ as follows.

- **ZINIT** If $h \in \mathcal{V}$, then $\hat{Z}^h$ is defined as in Setup B.2. We also set $\hat{Z}^h \overset{\text{def}}{=} Z^h$ and $\hat{\theta} \overset{\text{def}}{=} 0$.
- **ZNONLIN** Given $\psi : \mathbb{R}^k \times \mathbb{R}^l \to \mathbb{R}$, previous scalars $\theta_1, \ldots, \theta_i \in \mathbb{R}$ and vectors $x^1, \ldots, x^k \in \mathbb{R}^n$, we have
  \[ Z^{\psi(x)} \overset{\text{def}}{=} \psi(Z^{x^1}, \ldots, Z^{x^k}; \hat{\theta}_1, \ldots, \hat{\theta}_i). \]  
  (62)
- **ZMOMENT** Given same setup as above and scalar $\theta = \frac{1}{n} \sum^n_{\alpha=1} \theta(x^{\alpha}_1, \ldots, x^{\alpha}_k; \hat{\theta}_1, \ldots, \hat{\theta}_i)$, then
  \[ \hat{\theta} \overset{\text{def}}{=} \mathbb{E}(Z^{x^1}, \ldots, Z^{x^k}; \hat{\theta}_1, \ldots, \hat{\theta}_i). \]  
  (63)
  Here $\hat{\theta}_1, \ldots, \hat{\theta}_i$ are deterministic, so the expectation is taken over $Z^{x^1}, \ldots, Z^{x^k}$.

- **ZMATMUL** $Z^{Wx} \overset{\text{def}}{=} \hat{Z}^{Wx} + \hat{Z}^{Wx}$ for every matrix $W$ (with $\mathcal{N}(0, \sigma_W^2/n)$ entries) and vector $x$, where
  \[ \hat{Z}^{Wx} \]  
  is a Gaussian variable with zero mean. Let $\mathcal{V}_W$ denote the set of all vectors in the program of the form $W_x$ for some $y$. Then $\{\hat{Z}^{Wx} : W \in \mathcal{V}_W\}$ is defined to be jointly Gaussian with zero mean and covariance
  \[ \text{Cov} \left( \hat{Z}^{Wx}, \hat{Z}^{Wy} \right) \overset{\text{def}}{=} \sigma_W^2 \mathbb{E} Z^x Z^y, \quad \text{for any } W x, W y \in \mathcal{V}_W. \]  
  (64)
  Furthermore, $\{\hat{Z}^{Wx} : W \in \mathcal{V}_W\}$ is mutually independent from $\{\hat{Z}^v : v \in \mathcal{V} \cup \{A : A \in \mathcal{W}\}\}$, where $\mathcal{W}$ ranges over $\mathcal{V} \cup \{A : A \in \mathcal{W}\}$.

- **ZDOT** We can always unwind $Z^x = \Phi(\cdots)$, for some arguments $(\cdots) = ((\hat{Z}^{W^\top y_i})^k_{i=1}; (\hat{\theta}_i)^l_{i=1}; z^i \notin Y_{W^\top}(\text{where } Y_{W^\top} \text{ is defined in ZHAT}),$ and deterministic function $\Phi : \mathbb{R}^{k+j+l} \to \mathbb{R}$. Define $\partial Z^x / \partial Z^{W^\top y} \overset{\text{def}}{=} \partial_i \Phi(\cdots)$. Then we set
  \[ \hat{Z}^{Wx} \overset{\text{def}}{=} \sigma_W^2 \sum^k_{i=1} Z^{y_i} \mathbb{E} \frac{\partial Z^x}{\partial Z^{W^\top y}}, \]  
  (65)
  There is some nuance in this definition, so see Remark B.5 and B.6.

The following theorem ties the symbolic nature of the $Z$s to the analytic nature of a Tensor Program.

**Theorem B.4** (NETSOR$\uparrow$ Master Theorem, c.f. Theorem E.15 of (Yang, 2020b)). Fix a Tensor Program initialized accordingly to Setup B.2. Adopt Assumption B.8. Then

1. For any fixed $k$ and any pseudo-Lipschitz $\psi : \mathbb{R}^k \to \mathbb{R}$, as $n \to \infty$,
   \[ \frac{1}{n} \sum^n_{\alpha=1} \psi(h^{\alpha}_1, \ldots, h^{\alpha}_k) \overset{\text{a.s.}}{\longrightarrow} \mathbb{E}(\hat{Z}^{h_1}, \ldots, \hat{Z}^{h_k}), \]  
   (66)
   for any vectors $h_1, \ldots, h_k$ in the program, where $\hat{Z}^{h_i}$ are as defined in Definition B.3.

2. Any scalar $\theta$ in the program tends to $\hat{\theta}$ almost surely, where $\hat{\theta}$ is as defined in Definition B.3.
Remark B.5 (Partial derivative). The partial derivative in ZDOT should be interpreted as follows. By a simple inductive argument, $Z^x$ for every vector $x$ in the program is defined uniquely as a deterministic function $\varphi(\hat{Z}^{x_1}, \ldots, \hat{Z}^{x_k})$ of some $x_1, \ldots, x_k \in \mathcal{Y}$ or introduced by MatMul (notationally, we are suppressing the possible dependence on limit scalars $\theta_1, \ldots, \theta_l$). For instance, if in a program we have $A \in \mathcal{W}, v \in \mathcal{Y}, y = Av, x = A^T y$, then $Z^x = Z^z + Z^v$, so $\varphi$ is given by $\varphi(a, b) = a + b$. Then

$$\frac{\partial Z^x}{\partial \hat{Z}^{x^i}} \overset{\text{def}}{=} \partial_i \varphi(\hat{Z}^{x_1}, \ldots, \hat{Z}^{x_k}), \quad \text{and} \quad \frac{\partial Z^x}{\partial \hat{Z}^z} \overset{\text{def}}{=} 0 \text{ for any } z \not\in \{x_1, \ldots, x_k\}.$$

Note this definition depends on the precise way the program is written, not just on the underlying mathematics. For example, if $y, z \in \mathcal{Y}$ and $x = \varphi(W(y + z))$, then $Z^x = \varphi(\hat{Z}^{W(y+z)})$ so that $\partial Z^x / \partial \hat{Z}^{Wy} = \partial Z^x / \partial \hat{Z}^Wz = 0$. If instead, we have $x = \varphi(Wy + Wz)$, then $Z^x = \varphi(\hat{Z}^{Wy} + \hat{Z}^Wz)$ so that $\partial Z^x / \partial \hat{Z}^{Wy} = 0$. However, in both cases, $\hat{Z}^{Wy} = (W^T + W^T) \varphi'(W(y + z))$.

Remark B.6 (Partial derivative expectation). The quantity $\mathbb{E} \frac{\partial Z^x}{\partial \hat{Z}^{W^T y}}$ is well defined if $Z^x$ is differentiable in $\hat{Z}^{W^T y}$. However, even if this is not the case, e.g. if $x = \theta(W^T y)$ where $\theta$ is the heavyside step function, we can still define this expectation by leveraging Stein’s lemma:

In ZDOT, suppose $\{W^T y\}_{i=1}^k$ are all elements of $\mathcal{V}_{W^T}$ introduced before $x$. Define the matrix $C \in \mathbb{R}^{k \times k}$ by $C_{ij} \overset{\text{def}}{=} \mathbb{E} Z^{W^T} Y^{W^T} Z^x$ and define the vector $b \in \mathbb{R}^k$ by $b_i \overset{\text{def}}{=} \mathbb{E} \hat{Z}^{W^T} Y^{W^T} Z^x$. If $a = C^+ b$ (where $C^+$ denotes the pseudoinverse of $C$), then in ZDOT we may set

$$\sigma_x^2 \mathbb{E} \frac{\partial Z^x}{\partial \hat{Z}^{W^T y}} = a_i. \quad (67)$$

This definition agrees with the partial derivative expectation by Stein’s lemma when the latter is well defined. Theorem B.4 holds with this broader definition of partial derivative expectation.

**Pseudo-Lipschitz functions** are, roughly speaking, functions whose weak derivatives are polynomially bounded.

Definition B.7. A function $f : \mathbb{R}^k \rightarrow \mathbb{R}$ is called pseudo-Lipschitz of degree $d$ if $|f(x) − f(y)| \leq C\|x − y\|(1 + \sum_{i=1}^k |x_i|^d + |y_i|^d)$ for some $C$. We say $f$ is pseudo-Lipschitz if it is so for any degree.

Here are some basic properties of pseudo-Lipschitz functions:

- The norm $\|\cdot\|$ in Definition B.7 can be any norm equivalent to the $\ell_2$ norm, e.g. $\ell_p, p \geq 1$, norms. Similarly, $\sum_{i=1}^k |x_i|^d + |y_i|^d$ can be replaced by $\|x\|_p^d + \|y\|_p^d$ for any $p \geq 1$.
- A pseudo-Lipschitz function is polynomially bounded.
- A composition of pseudo-Lipschitz functions of degrees $d_1$ and $d_2$ is pseudo-Lipschitz of degree $d_1 + d_2$.
- A pseudo-Lipschitz function is Lipschitz on any compact set.

We adopt the following assumption for the Master Theorem Theorem B.4.

**Assumption B.8.** Suppose

1. If a function $\phi(\cdot : -) : \mathbb{R}^{0+l} \rightarrow \mathbb{R}$ with only parameter arguments is used in Moment, then $\phi$ is continuous in those arguments.

2. Any other function $\phi(\cdot ; -) : \mathbb{R}^{k+l} \rightarrow \mathbb{R}$ with parameters (where $k > 0$) used in Nonlin or Moment is pseudo-Lipschitz in all of its arguments (both inputs and parameters).

Statement 1 in Assumption B.8 essentially says that if we have scalars $\theta_1, \ldots, \theta_l$ in the program, then we can produce a new scalar by applying a continuous function (a weaker restriction than a pseudo-Lipschitz function) to them. Indeed, if $\theta_1, \ldots, \theta_l$ converge almost surely, then this new scalar does too. In our setting, statement 1 is used to allow any loss function whose derivative is continuous.

Other versions of the Master Theorem can be found in [Yang, 2020b], for example, versions where we do not assume any smoothness condition at all on the nonlinearities beyond that they be polynomially bounded, in exchange for assuming what’s called a rank stability condition. This rank stability should be generically true, but checking it rigorously is subtle, so we are content with the pseudo-Lipschitz condition in this paper.
C. More Diagrams

We can augment the graphical form of NETSOR $\top$ to accommodate the $\text{MOMENT}$ instruction in $\text{NETSOR}^\top$. See Fig. 4 for an example for layernorm and attention. In short, we denote scalar variables with a square, in contrast to the circle for vector variables, and we use a “bar-gate” to denote the $\text{MOMENT}$, where the function in the gate corresponds to $\psi$ in $\text{MOMENT}$.

In addition, for more examples of the expressivity of $\text{NETSOR}^\top$, Figs. 5 and 6 demonstrate convolution and MLP backpropagation in $\text{NETSOR}^\top$.

D. Proof of Main Result

We dedicate the following section to prove Theorem 5.3. We will begin by proving a simplified version under the same assumptions as Section 5.1, as reproduced below:

Setup D.1 (Representable NN in NTK Parametrization). Suppose a neural network $f \in \mathbb{R}$ is represented by a NETSOR $\top$ program (in the sense of Definition 4.2) whose $\text{NONLIN}$ all have polynomially bounded derivatives. Adopt the NTK parametrization: for every matrix parameter $W \in \mathbb{R}^{n \times n}$ of $f$, we factor $W = \frac{1}{\sqrt{n}} w$ where $w$ is the trainable parameter; likewise, for each input layer matrix $U^i \in \mathbb{R}^{n \times d}$, we factor $U^i = \frac{1}{\sqrt{d}} u^i$, and likewise the output matrix $V = \frac{1}{\sqrt{n}} v$. We randomly initialize all trainable parameters iid as $\mathcal{N}(0, 1)$. Furthermore, we assume the following:

A1. Input and output layers $\{u^i\}, v$, as well as biases are not trained (only $\mathbb{R}^{n \times n}$ weight matrices are trained).

A2. The forward pass does not use both a matrix and its transpose (in different $\text{MATMUL}$s).

27 More generally, we can allow any pseudo-Lipschitz function here, but for simplicity we go with the statement in the main text.
While conditioned on $f$, where $X$ is given by (see e.g. (Yang, 2020b, Sec K.2))
\[ f_1(\xi) \] converges almost surely to a random variable $\tilde{f}_1(\xi)$ as width $\to \infty$, such that
\[ \tilde{f}_{t+1}(\xi) - \tilde{f}_t(\xi) = -\tilde{K}(\xi, \xi)\mathcal{L}'_t(\tilde{f}_t(\xi)) \] (68)
where $\tilde{K}$ is the infinite-width NTK (at initialization) of the neural network.

**D.1. SGD as a NETSOR$^{+\top}$ Program**

SGD is comprised of a sequence of forward and backward passes computed on some architecture. WLOG, let $\pi_0$ denote the reduced program implementing the body of network $f$, and let $\xi(\xi)$ denote the final embedding such that $f(\xi) = V^T \xi(\xi)$, we will now show how the SGD procedure on $\pi_0$ can be implemented by a NETSOR$^{+\top}$ program.

**D.1.1. First Forward Pass**

While $\pi_0$ implements the embeddings $\xi(\xi)$ by definition, the outputs $f(\xi)$ cannot be implemented trivially in a program since that at initialization $f(\xi) = \frac{V^T \xi(\xi)}{\sqrt{n}}$ is not deterministic, and converges non-trivially to a GP, violating the requirements of a scalar type in a NETSOR$^{+\top}$ program which require all scalar types to converge to a deterministic limit as $n \to \infty$. Nevertheless, we can still easily express evolution of $f$ conditioned on (i.e. fixing) the values of $f$ at initialization. More formally, let $\mathbf{x} = [f(\xi_0), f(\xi_1), \ldots, f(\xi_D-1)]^\top \in \mathbb{R}^D$ denote a fixed vector of outputs, and let $X = [\xi(\xi_0), \xi(\xi_1), \ldots, \xi(\xi_D-1)]^\top \in \mathbb{R}^{n \times D}$ denote a fixed embedding matrix such that $\mathbf{f} = \frac{X^T \mathbf{x}}{\sqrt{n}}$. The distribution of $\mathbf{v}$ when conditioned on $\mathbf{x}$ and $X$ is given by (see e.g. (Yang, 2020b, Sec K.2))
\[ \mathbf{v} \overset{d}{=} \mathbf{f}_{\mathbf{x}}X^+ + \mathbf{PiV} \] (69)
where $X^+$ is the pseudo-inverse of $X$, $\mathbf{v}$ is an independent copy of $\mathbf{v}$ and $\mathbf{Pi}$ is the projection operator projecting unto the orthogonal complement of the space spanned by $X$. Namely:
\[ X^+ = \frac{1}{n}X \left( \frac{X^T X}{n} \right)^+, \quad \mathbf{Pi} = I - X^+X^\top \] (70)
Denote $\Sigma = \frac{X^T X}{n} \in \mathbb{R}^{D \times D}$, $\mu = \frac{X^T \mathbf{f}}{n} \in \mathbb{R}^D$. Define
\[ \hat{\mathbf{f}} \overset{d}{=} X \left( \frac{\Sigma^+ \mathbf{f}}{\sqrt{n}} \right) + \mathbf{v} - X\Sigma^+ \mu. \] (71)
Then we see via Eq. (69) that
\[ v \overset{d}{=} t, X \hat{v}. \] (72)

Given \( v \) and (the columns of) \( X \) as vectors and \( f \) as scalars in a program, \( \hat{v} \) may be defined in the same program via NONLIN, where \( \frac{\Sigma^t f}{\sqrt{n}} \) and \( \Sigma^t \mu \) (both finite-dimensional) provide coefficients for the linear combination over (columns of) \( X \). Formally, to express the evolution of \( f \) conditioned on \( f_0 = f \) at initialization, the program will calculate the first forward pass up to \( X \), calculate the loss derivatives \( \chi \) assuming \( f_0 = f \), and then proceed with the backward pass and later forward/backward passes with \( v \) replaced by \( \hat{v} \).

However, since \( \frac{\Sigma^t f}{\sqrt{n}}, \mu \overset{a.s.}{\longrightarrow} 0 \) and \( \Sigma^t \overset{a.s.}{\longrightarrow} \hat{\Sigma} \) (by rank stability, c.f. (Yang, 2020b, Lemma L.11)), these coefficients of the linear combination converge to 0, so that \( Z \overset{\hat{v}}{=}_{Z^*} \). Intuitively, this means that the distribution of \( v \) conditioned on the equality \( f = X^\top v/\sqrt{n} \) is asymptotically no conditioning as \( n \to \infty \). Thus, for the limit calculation of \( \delta f_t \) and other quantities, it ends up not mattering whether we use \( \hat{v} \) or \( v \).

**Computing The Loss Derivatives** The loss derivative \( \chi(\xi) = \frac{\partial L(f(\xi))}{\partial f(\xi)} \) after the first forward pass given \( f(\xi) \) can be implemented with MOMENT instructions using \( \psi(f(\xi)) = L'(f(\xi)) \).

**D.1.2. Implementing SGD**

Under SGD, the update at step \( t + 1 \) to any weight \( w \in \mathbb{R}^{n \times n} \) is given by:
\[
 w_{t+1} - w_t = -\chi_t \sum_{g,h:e=Wt} \frac{dg_t h_t^\top}{n}, 
\] (73)

where the summation in Eq. (73) is over all pairs of vectors \( g, h \) in program \( \pi_0 \) satisfying \( g = Wh \) (there can be multiple such pairs since \( \pi_0 \) may reuse the same matrix \( W \)).

To write the full unrolled SGD as a NETSOR\( \top^{+} \) program, we will need to implement the error signal \( dg_t \overset{df}{=} \sqrt{n} \frac{\partial f_t}{\partial p_t} \) for each G-var \( g \) at time \( t \). To accomplish this, we recall the notion of paths in program \( \pi_0 \):

**Definition 5.5 (Paths).** In a NETSOR\( \top^{+} \) program, a path \( p \) starts with an X-var and ends with a G-var, alternating between X- and G-vars along the path. We write \( p^{\prime} \) for the starting X-var, \( p^{\dagger} \) for the following G-var, and so on, as well as \( p^{-1} \) for the ending G-var (see Fig. 2 for a graphical illustration). For odd \( i \), let \( W^p \) denote the defining matrix of G-var \( p^i \). For two equal length paths \( p, q \), we write \( p \equiv q \) (path \( p \) is isomorphic to path \( q \)) if for all odd \( i \), \( W^p^i \) is the same matrix as \( W^q^i \).28 In other words, we say path \( p \) is isomorphic to path \( q \) if their sequences of MATMUL matrices are identical, (but the NONLIN don’t have to be, see Fig. 3 for a graphical illustration). Let \( |p| \) denote the number of vectors in \( p \) (this is always an even number).

Note that a path \( p \) represents a series of nodes independent of an input, and can be instantiated as \( p(\xi) \) by an input \( \xi \), resulting in a series of instantiated G-vars and X-vars \( p^i(\xi) \).

For any G-var \( g = Wh \), we can write the error term \( dg \) as the summation of errors signals over paths \( p \):
\[
dg(\xi) = \sum_{p, p^{-1} = x \ldots p^1 = g} J_p(\xi) \]
(74)

where \( J_p = \left( \frac{\partial p^2}{\partial p^1} \right)^\top \left( \frac{\partial p^1}{\partial p^{-2}} \right)^\top \left( \frac{\partial p^{-1}}{\partial p^{-2}} \right)^\top v \) (75)

(Here again, \( J_p \) represents a symbolic computation that can be instantiated with an input \( J_p(\xi) \)). Note that \( J_p \) can be defined recursively:
\[
 J_p = \left( \frac{\partial p^2}{\partial p^1} \right)^\top \left( \frac{\partial p^3}{\partial p^2} \right)^\top \frac{\partial p^{-3}}{\partial p^{-2}} J_p^{\geq 3} 
\]
(76)

28Here we are talking about equality of symbols rather than equality of values of those symbols.
where \( J_{p,k} \), \( k \leq |p| \) is defined as:

\[
J_{p,k} \overset{\text{def}}{=} \left\{ \left( \frac{\partial p^{k+1}}{\partial p^k} \right)^\top \left( \frac{\partial p^{k-1}}{\partial p^k} \right)^\top \ldots \left( \frac{\partial p^1}{\partial p^k} \right)^\top v \right\} \ k \leq |p| \\
\ k \geq |p| 
\]

(77)

Recall that each path \( p \) starts with an X-var \( p^0 \), and alternates between G and X vars. Let \( W^p \) denote the defining weight matrix of G-var \( p^3 \) (i.e. \( p^3 = W^p p^2 \)), and let \( p^2 = \psi(...,p^1,...) \). Then we can re-write Eq. (76) as:

\[
J^p = \psi(...,p^1,...) \odot J^{p^2}, \quad J^{p^2} = (W^p)^\top J^{p^3}
\]

(78)

Note that Eq. (78) can be written in NETSOR\( ^\top \) language using MATMUL instructions using the transposed weights, and NONLIN instructions using \( \psi' \), which is pseudo-Lipschitz by Setup D.1.

Recall that \( \pi_0 \) is the program defining the network architecture. We now write the unrolled SGD of this network in a new program \( \pi \). Below, recall that lack of time subscript means \( t = 0 \) (e.g. \( W \) means \( W_0 \), the initialized value). In addition, feel free to revisit the notations explained before Appendix A.

- If \( g = Wh \in \pi_0 \), then:

\[
\delta \tilde{g}_{t+1} = \sqrt{n}(W_{t+1} \tilde{h}_{t+1} - W_t \tilde{h}_t) = W \tilde{\delta}h_{t+1} + \sqrt{n}(W_{t+1} - W_t) \tilde{h}_t + \sum_{s=0}^{t}(W_{s+1} - W_s) \delta \tilde{h}_{t+1}
\]

(79)

where, using Eq. (73), we have

\[
\sqrt{n}(W_{t+1} - W_t) \tilde{h}_t = -\chi_t \sum_{g,h:g=W_{h}} dg_t \frac{h_t^\top \tilde{h}_t}{n}
\]

(80)

\[
\sum_{s=0}^{t}(W_{s+1} - W_s) \delta \tilde{h}_{t+1} = -\sum_{s=0}^{t} \chi_s \sum_{g,h:g=W_{h}} dg_s \frac{h_s^\top \delta \tilde{h}_t}{n}
\]

(81)

**Tensor Program implementation**  Eqs. (79) to (81) may be easily implemented using NETSOR\( ^\top \) + instructions. For instance, Eq. (80) (assuming the sum sums over a single pair \( \{h,g\} \)) may be implemented using MOMENT and NONLIN instructions as follows: the term \( \frac{h_t^\top \tilde{h}_t}{n} \) may be implemented by a MOMENT instruction with \( \psi(\tilde{h}_t, h_t) = \frac{1}{n} \sum_{\alpha}(\tilde{h}_t)_{\alpha}(h_t)_{\alpha} \). The full term is then a NONLIN + instructions \( \psi(dg_t; \chi_t, \{\frac{h_t^\top \tilde{h}_t}{n}\}) \) with scalars \( \chi_t \), \( \{\frac{h_t^\top \tilde{h}_t}{n}\} \) and vector \( dg_t \).

- If \( g = \psi(h^1, ..., h^k) \in \pi_0 \), then

\[
\delta \tilde{g}_{t+1} = \sqrt{n} \left( \psi(\tilde{h}_1^1, \frac{\tilde{h}_1^1}{\sqrt{n}}, ..., \tilde{h}_k^k, \frac{\tilde{h}_k^1}{\sqrt{n}}) - \psi(\tilde{h}_1^1, ..., \tilde{h}_k^k) \right).
\]

(82)

**Tensor Program implementation**  Eq. (82) may be implemented as a NONLIN + instruction:

\[
\delta \tilde{g}_{t+1} := \psi^* \left( \frac{\{\tilde{h}_1^1\}_{i=1}^k \cup \{\delta \tilde{h}_i^{i+1}\}_{i=1}^k}{\sqrt{n}} \right)
\]

(83)

for a set of vectors \( \{\tilde{h}_1^{i}\}_{i=1}^k \), \( \{\delta \tilde{h}_i^{i+1}\}_{i=1}^k \) and a scalar \( \frac{1}{\sqrt{n}} \), where:

\[
\psi^* (\{\mu^i\}_{i=1}^k \cup \{\nu^i\}_{i=1}^k, \theta) \overset{\text{def}}{=} \left\{ \begin{array}{ll}
\psi(\mu^1 + \theta \nu^1, ..., \mu^k + \theta \nu^k)_{\alpha} - \psi(\mu^1, ..., \mu^k)_{\alpha} & \theta > 0 \\
\sum_{i=1}^k \frac{\partial \psi(\mu^1, ..., \mu^k)}{\partial \mu^i} \nu^i_{\alpha} & \theta = 0
\end{array} \right.
\]

(84)

Since \( \psi^* \) is pseudo-Lipschitz by Setup D.1, \( \psi^* \) is pseudo-Lipschitz in all of its inputs as well.

- WLOG assume \( f(\xi) = \frac{\psi(\xi)}{\sqrt{n}} \), then:

\[
\tilde{f}_{t+1} = \frac{\psi^\top \delta \tilde{g}_{t+1}}{n}, \quad \chi_t = \nabla f_t \mathcal{L}_t.
\]

(85)
Algorithm 1

Tensor Program implementation the scalar type outputs $f_t(\xi)$ at $t > 0$ for any input $\xi$ can be implemented using the \texttt{MOMENT} instruction. The loss derivative $\chi_t, t > 0$ given $f_t$ can be implemented with \texttt{MOMENT} instructions using $\psi(-; f_t(\xi)) = \mathcal{L}'(f_t(\xi))$ where $f(\xi)$ is treated as a scalar type as in the first forward pass.

• If $g \in \mathbb{R}^n \in \pi_0$:

$$ g_{t+1}(\xi) = g(\xi) + \frac{1}{\sqrt{n}} \sum_{s=1}^{t+1} \delta g_s(\xi) \quad (86) $$

Tensor Program implementation $\delta g_{t+1}$ is implemented using a \texttt{NONLIN} instruction $g_{t+1}(\xi) = \psi(g(\xi) \cup \{\delta g_s(\xi)\}_{s=1}^{t+1}; \theta) = \mu + \theta \sum_s \nu_s$.

• If $g = Wh \in \pi_0$, then using Eq. (74):

$$ dg(\xi)_{t+1} = \sum_{p:p^t = x, p^t = g} J^p_{t+1}(\xi) \quad (87) $$

$$ J^p_{t+1} = \psi'(..., p^1_{t+1}, ...) \odot (\{W^p_{t+1}\} \cdot J^p_{t+1}) \quad (88) $$

Using Eq. (76), $J^p_{t+1}$ is implemented recursively starting from $J^{p-2}_{t+1} = (W^{-1}_{t+1})^\top v$. Plugging in the weights update at time $t + 1$ (Appendix D.1.2):

$$ J^{p-2}_{t+1} = (W^{-1}_{t} + W^{-1}_{t} - W^{-1}_{t} )^\top v = J^{p-2}_{t} - \chi_t \sum_{g,h: g = W_{t+1}^{-1} h} h_t \frac{dg^\top}{n} \quad (89) $$

$$ J^p_{t+1} = \psi'(..., p^1_{t} + \frac{\delta p^1_{t+1}}{\sqrt{n}}, ...) \odot J^p_{t+1} \quad (90) $$

Tensor Program implementation $dg(\xi)_{t+1}$ is implemented using \texttt{MOMENT} and \texttt{NONLIN} instructions.

For further illustration, we present in Algorithm 1 a program implementation of the first iteration of SGD on the two hidden layer MLP specified in Appendix A.2, but where only the middle layer $w$ is trained; in Fig. 7 we have its graphical form. Naturally, the following SGD steps can be implemented in a similar fashion.

\begin{algorithm}
\caption{\texttt{NETSOR} $^+$ program $\pi_1$ implementing the first update $\tilde{f}_1 - \tilde{f}$. Note that in this example, $\psi$ represents multiple functions, while $\phi$ is a fixed function representing the non-linearity of the MLP in Appendix A.2. Technically, we should have $\tilde{v}$ as defined in Appendix D.1.1 instead of $\tilde{v}$, but as explained there, this does not affect the limit.

\textbf{Input: } $\mathcal{W} = \{w\}, \mathcal{V} = \{v, g = g_0(\xi_0), \tilde{g} = g_0(\tilde{\xi})\}, \mathcal{C} = \{f = f_0(\xi_0), \tilde{f} = f_0(\tilde{\xi})\}$
\textbf{MOMENT: } $\chi := \mathcal{L}'(f)$
\textbf{NONLIN} $^+$: $z := \phi(g)$
\textbf{NONLIN} $^+$: $\tilde{z} := \phi(\tilde{g})$
\textbf{MATMUL: } $h := W g$
\textbf{MATMUL: } $\tilde{h} := W \tilde{g}$
\textbf{NONLIN} $^+$: $\tilde{z} := \phi(\tilde{g})$
\textbf{MOMENT: } $\theta := \psi(z, \tilde{z}) = \frac{z + \tilde{z}}{2}$
\textbf{NONLIN: } $dh := \psi(v, h) = \phi(h) \odot v$
\textbf{NONLIN} $^+$: $\delta h_1 := \psi(v, h; \theta, \chi) = -\chi \theta dh$
\textbf{NONLIN} $^+$: $\delta \tilde{h}_1 := \psi(\tilde{v}, \tilde{h}; \theta, \chi) = -\chi \theta \tilde{d}h$
\textbf{MOMENT: } $\tilde{f}_1 - \tilde{f} = \frac{w \delta \tilde{z}}{n}$
\textbf{Output: } $\tilde{f}_1 - \tilde{f}$
\end{algorithm}
SGD in the Infinite Width Limit  
According to the NETSOR $\mathcal{T}^+$ rules as specified in Definition B.3, we have the following identities:

- If $g = Wh$, then using Eqs. (79) to (81): (Here $Z^d_{8t} = Z^d_{8t}(\xi_i), Z^h_{8t} = Z^h_{8t}(\xi_i)$, and $Z^k = Z^h(\xi)$)

$$Z^d_{8t+1} = Z^d_{8t+1} - \chi_t \sum_{g,h} E[Z^h g Z^k]$$

where

$$Z^d_{8t+1} = Z^d_{8t+1} + \sum_{y} Z^y E \frac{\partial Z^h_{8t+1}}{\partial Z^y_{8t+1}}.$$  

- If $g = \psi(h^1, \ldots, h^k)$, then using Eqs. (82) and (84), taking the limit $1/\sqrt{n} \to 0$,

$$Z^d_{8t+1} = \sum_{i=1}^{k} \frac{\partial \psi(Z^h_{8t}, \ldots, Z^h_{8t})}{\partial Z^i_{8t}} Z^h_{8t+1}.$$  

- Using Eqs. (86), (87), (89) and (90) and taking $1/\sqrt{n} \to 0$, we have by $\text{ZNONLIN}^+$:

$$Z^0_{8t}(\xi) = Z^0_{8t}(\xi), \quad Z^{d0}_{8t}(\xi) = Z^{d0}_{8t}(\xi) \quad \text{for any vector } g \in \pi_0 \text{ at time } t.$$  

D.2. Deriving The NTK

Instantiate paths $p$ and $q$ on two inputs $\xi, \xi'$ by $p = p(\xi), q = q(\xi')$ (abusing notation slightly). We define an inner product between them as follows:

$$\langle p, q \rangle \equiv E[Z^p Z^q] \prod_{i=2,\text{even}}^{|p|-2} E \left[ \frac{\partial Z^i}{\partial Z^{p_{i-1}}} \frac{\partial Z^i}{\partial Z^{q_{i-1}}} \right].$$  

where $p^i, q^i$ are X-vars for all even $i$. Note that for even $i$, $p^i$ is always of the form $p^i = \psi(\ldots, p^{i-1}, \ldots)$ for some $\psi$. So the partial derivatives in Eq. (95) are just $\frac{\partial Z^i}{\partial Z^{p_{i-1}}(\xi)} = \psi'(\ldots, Z^{p_{i-1}}, \ldots)$.

Our goal in this section is to prove...
Applying this logic recursively, we have

\[
\bar{\psi}(\xi, \hat{\xi}) = \sum_{p,q: p^{-1} = q^{-1} = x, p \neq q} \langle p(\xi), q(\hat{\xi}) \rangle. 
\] (96)

For each weight \( W \in \mathcal{W} \), the gradient of the output with respect to \( w \) is given by:

\[
\nabla_w f(\xi) = \sum_{g, h: g = Wh} \frac{dg(\xi) h(\xi)^\top}{n} 
\] (97)

Here, \( g, h \) represent nodes in program \( \pi_0 \) that can be instantiated by an input \( \xi \).

The NTK of \( f \) can be expressed as:

\[
\bar{\mathcal{K}}(\xi, \hat{\xi}) = \lim_{n \to \infty} \sum_{W \in \mathcal{W}} \langle \nabla_w f(\xi), \nabla_w f(\hat{\xi}) \rangle = \lim_{n \to \infty} \sum_{W \in \mathcal{W}} \sum_{g, h: g = Wh} \frac{dg(\xi) h(\xi)^\top h(\hat{\xi})}{n} 
\] (98)

\[
= \sum_{W \in \mathcal{W}} \sum_{g, h: g = Wh} \mathbb{E} \left[ Z_{dg(\xi)} Z_{dg(\hat{\xi})} \right] \mathbb{E} \left[ Z_{h(\xi)} Z_{h(\hat{\xi})} \right]. 
\] (99)

Using Eqs. (74) and (78), for any G-var \( g = Wh \), we can write the error term \( dg \) as the summation of errors signals over paths \( p \):

\[
dg(\xi) = \sum_{p: p^{-1} = x, p^1 = g} J_p(\xi), \quad J_p = \psi'(\ldots, p^1, \ldots) \circ ((W_p^3)^\top J_p^3) 
\] (100)

Hence we can write:

\[
\mathbb{E} \left[ Z_{dg(\xi)} Z_{dg(\hat{\xi})} \right] = \sum_{p^1 = g, p^{-1} = x, q^1 = g, q^{-1} = x} \mathbb{E} \left[ Z_{J_p^1(\xi)} Z_{J_q^1(\hat{\xi})} \right] = Z_{J_p^p} = Z(W_p^3)^\top J_p^3 \frac{\partial Z_{p^2}^p}{\partial Z_{p^3}} 
\] (101)

where \( \psi' \) denotes the derivative w.r.t. \( p^1 \). By Simple GIA Check (Yang, 2020a), we have that \( Z(W_p^3)^\top J_p^3 = \hat{Z}(W_p^3)^\top J_p^3 \) (see ZMATMUL). Hence, with abuse of notation \( J_p = J_p^p, J_q = J_q^q, p = p(\xi), q = q(\hat{\xi}) \), we have

\[
\mathbb{E} \left[ Z_{J_p^p} Z_{J_q^q} \right] = \mathbb{E}[\hat{Z}(W_p^3)^\top J_p^p \hat{Z}(W_q^3)^\top J_q^q] \mathbb{E}[\frac{\partial Z_{p^2}^p}{\partial Z_{p^3}} \frac{\partial Z_{q^2}^q}{\partial Z_{q^3}}]. 
\] (102)

From the definition of \( \hat{Z} \), the expectation \( E[\hat{Z}(W_p^3)^\top J_p^p \hat{Z}(W_q^3)^\top J_q^q] \) vanishes if the weights \( W_p^3 \) and \( W_q^3 \) are not symbolically the same (i.e \( W_p^3 \not\equiv W_q^3 \)). Then by \( \hat{Z} \),

\[
\mathbb{E}[\hat{Z}(W_p^3)^\top J_p^p \hat{Z}(W_q^3)^\top J_q^q] = \begin{cases} 
\mathbb{E}[Z_{J_p^p} Z_{J_q^q}] & \text{if } W_p^3 \not\equiv W_q^3 \\
0 & \text{otherwise.}
\end{cases} 
\] (103)

Applying this logic recursively, we have

\[
\mathbb{E} \left[ Z_{J_p^p} Z_{J_q^q} \right] = \begin{cases} 
\prod_{i=1}^{\lceil p/2 \rceil} \mathbb{E} \left[ \frac{\partial Z_{p^i}^p}{\partial Z_{p^{i+1}}} \frac{\partial Z_{q^i}^q}{\partial Z_{q^{i+1}}} \right] & \text{if } p \not\equiv q \\
0 & \text{otherwise.}
\end{cases} 
\] (104)

Combining with Eqs. (74), (100) and (102) proves Proposition D.3.
D.3. Getting Claim 3.1

Notation For the remainder of the proof we abbreviate \( p = p(\hat{\xi}), q = q(\xi), p^i = p^i(\hat{\xi}), q^i = q^i(\xi) \) (i.e. path \( p \) is always evaluated on \( \hat{\xi} \), while path \( q \) is always evaluated on \( \xi \)). We prove Claim 3.1 by inducting on all G-vars in the network. We begin by proving the following induction hypothesis.

**Definition D.4.** We write \( Z^x \equiv Z^y \mod \hat{Z}^W \) to denote that \( Z^x - Z^y \) is a linear combination of \( \hat{Z}^W u \) for various vectors \( u \).

**Induction Hypothesis.** At any time \( t \) and G-var \( g = Wh \), the following holds:

\[
Z^{\hat{\delta}_{\hat{t}+1}} = -\chi_t \sum_{p:p^{-1}=g} \sum_{q:p=q} Z^{dq^{-1}} (p, q) \mod \hat{Z}^W
\]  

(107)

Here, the sum is over all paths \( p \) with endpoint \( g \) and all paths \( q \) isomorphic to \( p \). Recall that \( dq^{-1} \) is the (scaled) gradient \( dy \) where \( y = q^{-1} \) is the endpoint of \( q \).

D.3.1. Base Case

For initial G-vars \( g, \hat{\delta}_t = 0 \) since we are not training the input layers (Assumption A1.). This proves the base case since the sum in Eq. (107) has no terms and thus is 0.

D.3.2. Inductive Case

Suppose \( g = Wh \), where \( h = \psi(h^1, ..., h^k) \), we then have using Eq. (91):

\[
Z^{\hat{\delta}_{\hat{t}+1}} = \hat{Z}^{Wh_{\hat{t}+1}} + \chi_t \sum_{g=Wh} Z^{dg_W} E[Z^{h_W} \hat{Z}^h] \mod \hat{Z}^W
\]  

where \( \hat{Z}^{Wh_{\hat{t}+1}} = \sum_y Z^y E[\frac{\partial Z^{\delta_{\hat{h}_{t+1}}}}{\partial Z^{Wh_{t+1}}}] \).  

(109)

Note \( \sum_{g=Wh} Z^{dg_W} E[Z^{h_W} \hat{Z}^h] \) in Eq. (108) can be written as \( \sum_{p:p^{-1}=g, |p|=2} \sum_{q:q=p} Z^{dq^{-1}} (p, q) \). Therefore, it suffices to show that

\[
Z^{Wh_{\hat{t}+1}} = -\chi_t \sum_{p:p^{-1}=g, |p| \geq 2} \sum_{q:q \equiv p} Z^{dq^{-1}} (p, q).
\]  

(110)

**Showing Eq. (110)** By Eq. (82):

\[
Z^{\delta_{h_{t+1}}} = \sum_{i=1}^k \frac{\partial Z^h}{\partial Z^{h^i}} Z^{\delta_{h_{t+1}}^i}
\]  

(111)

Since \( Z^{h^1}, ..., Z^{h^k} \) do not depend on \( Z^{W^\top} y \) for any \( y \) (by the assumption that we don’t use both a matrix and its transpose in the forward pass), from Eq. (111) we have for any \( y \):

\[
E[\frac{\partial Z^{\delta_{h_{t+1}}}}{\partial Z^{Wh_{t+1}}}] = \sum_{i=1}^k E[\frac{\partial Z^h}{\partial Z^{h^i}} \frac{\partial Z^{\delta_{h_{t+1}}^i}}{\partial Z^{Wh_{t+1}}}].
\]  

(112)

Applying the induction hypothesis Eq. (107) to each G-var \( h^i \), we get

\[
\frac{\partial Z^{\hat{\delta}_{h_{t+1}}^i}}{\partial Z^{Wh_{t+1}} y} = -\chi_t \sum_{p:p^{-1}=h^i, q:q=p} \sum_{q:q=p} \frac{\partial Z^{dq^{-1}}}{\partial Z^{Wh_{t+1}} y} (p, q) \mod \hat{Z}^W
\]  

(113)

Plugging this back into \( \hat{Z}^{Wh_{\hat{t}+1}} \) (Eq. (109)), we get

\[
\hat{Z}^{Wh_{\hat{t}+1}} = -\chi_t \sum_y Z^y \sum_{i=1}^k \sum_{p:p^{-1}=h^i, q:q=p} (p, q) E[\frac{\partial Z^h}{\partial Z^{h^i}} \frac{\partial Z^{dq^{-1}}}{\partial Z^{Wh_{t+1}} y}].
\]  

(114)
Note that for any path $p$ with $p^{-1} = h^i$, we may extend $p$ by vectors $g, h$ (recall $g = Wh$ and $h = \psi(h^1, ..., h^k)$). Let $q$ denote this extension. If $q$ is a path such that

$$q \equiv p \text{ and } \frac{\partial Z_{dq^{-1}y}}{\partial Z_{W^T y}} = 1,$$

we have

$$\langle p, q \rangle \mathbb{E} \left[ \frac{\partial Z_h}{\partial Z_k} \frac{\partial Z_{dq^{-1}}}{\partial Z_{W^T y^j}} \right] = \langle p, q \rangle.$$  \hspace{1cm} (116)

Our goal now is to show $q$ in Eq. (114) can be extended appropriately such that we may rewrite Eq. (114) as Eq. (110). This will be done through explicitly computing the term $\frac{\partial Z_{dq^{-1}}}{\partial Z_{W^T y}}$ in Eq. (114).

**Computing $\frac{\partial Z_{dq^{-1}}}{\partial Z_{W^T y}}$** Suppose $\{g^1, ..., g^r\}$ are all G-vars in the program $\pi_0$ that depend on $q^{-1}$ i.e for all $1 \leq j \leq r$, we have $g^j = W^j y^j$ where $y^j = \psi_j(..., q^{-1}, ...)$ and where $W^j$ can be same or different matrices for different $j$. Note that it follows that:

$$dq^{-1} = \sum_{j=1}^r \psi_j(..., q^{-1}, ...) \odot ((W^j)^T dg^j)$$ \hspace{1cm} (117)

$$Z_{dq^{-1}} = \sum_{j=1}^r \frac{\partial Z_{y^j}}{\partial Z_{W^T y^j}} Z^{(W^j)^T dg^j}$$ \hspace{1cm} (118)

where $Z^{(W^j)^T dg^j} = \hat{Z}^{(W^j)^T dg^j} + \dot{Z}^{(W^j)^T dg^j} = \hat{Z}^{(W^j)^T dg^j}$. \hspace{1cm} (119)

Note that $\hat{Z}^{(W^j)^T dg^j} = 0$ in Eq. (119) from the gradient independence assumption (GIA) because we pass the Simple GIA Check. This may also be easily verified by explicitly computing $\hat{Z}^{(W^j)^T dg^j}$, and noticing that the expectation vanishes from the dependency of $Z_{dq^j}$ on $Z^v$ (i.e $Z_{dq^j} = Z^v Z^u$ for some vector $\mu$ which does not depend on $v$). Since $y$ does not depend on $v$ and the last layer $v$ is not trained, we have $\mathbb{E} \frac{\partial Z_{dq^j}}{\partial Z_{W^T y}} = \mathbb{E}[Z^v] \mathbb{E}[...] = 0$.

Since we assumed that the forward propagation does not contain both $W, W^T$, it follows from differentiating Eq. (118) that

$$\frac{\partial Z_{dq^{-1}}}{\partial Z_{W^T y}} = \sum_{j=1}^r \frac{\partial Z_{y^j}}{\partial Z_{W^T y}} \frac{\partial \hat{Z}^{(W^j)^T dg^j}}{\partial Z_{W^T y}} = \sum_{j:W^j \neq W, dg^j \neq y} \frac{\partial Z_{y^j}}{\partial Z_{W^T y}}.$$ \hspace{1cm} (120)

If this sum over $j$ is nonempty, then there is a unique $j$ such that $W^j \neq W$ and $dg^j = y$. In such a case, we may extend the path $q$ with $g^j, z^j$ to form $q$ satisfying Eq. (115). Plugging back into Eq. (114) we obtain Eq. (110) as desired.

Hence, we have proven the induction hypothesis.

### D.3.3. Proving Claim 3.1 Using the Induction Hypothesis

WLOG assume $f(\xi) = V^T x(\xi)$ for some G-var $x(\xi)$. Using the induction hypothesis and the Master Theorem (Theorem B.4), we have that:

$$\lim_{n \to \infty} \hat{f}_{t+1} - \hat{f}_t = \mathbb{E} Z^v Z^{\delta x_{t+1}} = -\chi_t \sum_{p:p^{-1} = x} \sum_{q : q \neq p} \mathbb{E} [Z^v Z_{dq^{-1}}] \langle p, q \rangle.$$ \hspace{1cm} (121)

Note that $Z_{dq^{-1}} = Z^v$ for any path $q : q^{-1} = x$. Hence, with Eq. (96), we have

$$\lim_{n \to \infty} \hat{f}_{t+1} - \hat{f}_t = -\chi_t \sum_{p:p^{-1} = x} \sum_{q : q \neq p} \langle p, q \rangle = -\chi_t \tilde{K}(\xi_t, \tilde{c})$$ \hspace{1cm} (122)

as desired.
D.4. Relaxing Assumptions (A1.) to (A4.)

We now briefly discuss the case where Assumptions (A1.) to (A4.) are relaxed, as well as the case where $f$ is represented by a NETSOR $T^+$ program. As the proof of the general case follows roughly the same logic as in Setup D.1, we only discuss the meaningful differences in each case.

D.4.1. Training the First and Last Layers

Recall the input and output layers are parameterized by $\{u^i\}, v$ which now depend on $t$. The output evolution is now given by:

$$
\tilde{f}_{t+1} - \tilde{f}_t = V_t^T \tilde{x}_{t+1} - V_t^T \tilde{x}_t = \frac{v^T \delta \tilde{x}_{t+1}}{n} + \frac{\sqrt{n}(v_{t+1} - v_t)^T \tilde{x}_t}{n} + \sum_{s=0}^{t} \frac{(v_{s+1} - v_s)^T \delta \tilde{x}_{t+1}}{n}.
$$

(123)

Plugging $v_{t+1} - v_t = -\chi t \frac{1}{\sqrt{n}} x_t$ into Eq. (123) and taking the limit (using NETSOR $T^+$ rules):

$$
\lim_{n \to \infty} \tilde{f}_{t+1} - \tilde{f}_t = E \left[ Z^v Z^{\delta \tilde{x}_{t+1}} \right] - \chi t E \left[ Z^{\tilde{x}(\xi)} Z_{\tilde{x}} \right].
$$

(124)

Evaluating $E \left[ Z^v Z^{\delta \tilde{x}_{t+1}} \right]$ by induction requires altering the path definition so that each path $p$ may start with an input $\xi$, and ends with a G-var (that is, a path either starts with an X-var or an input). We reuse the definition of inner product between $p \cong q$ in Eq. (95), only when both start with inputs $\xi, \xi$ respectively then $E \left[ Z^v Z^q \right]$ implies $\xi^T \xi$. The remainder of the proof follows the same logic as with Setup D.1. Note that the NTK in this case would yield:

$$
\tilde{K}(\xi, \tilde{\xi}) = \sum_{q \cong \tilde{\xi}} \langle p, q \rangle + E \left[ Z^{\tilde{x}(\xi)} Z_{\tilde{x}} \right].
$$

(125)

D.4.2. $W, W^T$ in the Forward Pass

When both $W, W^T$ are allowed in the forward pass, the update equations for each $w_t$ take the form:

$$
w_{t+1} - w_t = -\chi t \sum_{g, h, g = W h} d^g h^T \frac{n}{n} - \chi t \sum_{g, h, g = W^T h} h^T d^g \frac{n}{n}
$$

(126)

Some quick calculations using NETSOR $T^+$ rules show that for G-vars:

- If $g = Wh$:

$$
Z^{\delta \tilde{g}_{t+1}} = Z^{W \delta \tilde{h}_{t+1}} - \chi t \sum_{g, h, g = W h} Z^{dg(\xi)} E \left[ Z^{dh(\xi)} Z_{\tilde{h}} \right] - \chi t \sum_{g, h, g = W^T h} Z^{bh(\xi)} E \left[ Z^{dg(\xi)} Z_{\tilde{h}} \right].
$$

(127)

- If $g = W^T h$:

$$
Z^{\delta \tilde{g}_{t+1}} = Z^{W^T \delta \tilde{h}_{t+1}} - \chi t \sum_{g, h, g = W^T h} Z^{dg(\xi)} E \left[ Z^{dh(\xi)} Z_{\tilde{h}} \right] - \chi t \sum_{g, h, g = W h} Z^{bh(\xi)} E \left[ Z^{dg(\xi)} Z_{\tilde{h}} \right].
$$

(128)

It is straightforward to show using GIA (Yang, 2020a) that $E \left[ Z^{dg(\xi)} Z_{\tilde{h}} \right] = 0$ in both cases, leaving us with a similar expression as with Setup D.1. The induction hypothesis for G-vars in this case takes one of two forms:

- If $g = Wh$ then Eq. (107) holds.

- If $g = W^T h$ then Eq. (107) holds with $mod \tilde{Z}^{W^T *}$ replacing $mod \tilde{Z}^W *$.

Some additional complications need to be resolved. Specifically, with setup Setup D.1 we have used in two places the fact that no transpose is used in the forward pass to prove the induction hypothesis (see Eqs. (112) and (120)). To prove the induction, and assuming $g = Wh$, we now have instead of Eq. (112) (using Eq. (111)):

$$
E \frac{\partial Z^{\tilde{h}_{t+1}}}{\partial Z_{W^T} y} = \sum_{i=1}^{k} E \left[ \frac{\partial Z^h}{\partial Z^h} \frac{\partial Z^{\tilde{h}_{t+1}}}{\partial Z_{W^T} y} \right] + \sum_{i=1}^{k} E \left[ \frac{\partial^2 Z^h}{\partial Z^h \partial Z_{W^T} y} Z^{\tilde{h}_{t+1}} \right].
$$

(129)
We assumed in our proof that \( x \). We have used a scalar output and a batchsize of 1 throughout this paper. However, extending to multiple (finite) outputs
\[
\{ \sqrt{1} \}
\]
Therefore, we can treat any scalar produced through \( \mathcal{M} \) nonlinearities where the parameters are fixed). Then the same reasoning follows.

Using GIA (Yang, 2020a), it is straightforward to show that the expectation on the RHS of Eq. (130) vanishes, leaving us with the first term on the RHS of Eq. (129), as with Setup D.1. Note that the same logic may be applied in Eq. (120), concluding the proof.

### D.4.3. Multiple Outputs and Arbitrary Batchsize

We have used a scalar output and a batchsize of 1 throughout this paper. However, extending to multiple (finite) outputs and an arbitrary batchsize requires no additional arguments besides some additional notations. For example, the definition of path should now be altered to express dependency on multiple samples (if batchnorm is used for example). The proof however follows roughly the same logic in Setup D.1.

### D.4.4. X-var Embedding

We assumed in our proof that \( x \), which represents the final embedding of \( f \) is a G-var. However, extending the proof to the case where \( x \) is an X-var is straightforward. Let \( f(x) = V^T x(x) \) where \( x = \psi(h^1, \ldots, h^k) \) and \( h^1, \ldots, h^k \) are G-vars. Using the induction hypothesis, along with Eq. (93) yields:

\[
\lim_{n \to \infty} \hat{f}_{t+1} - \hat{f}_t = -\chi_t \mathbb{E} \left[ Z^v Z^\delta \right] = -\chi_t \sum_{i=1}^k \mathbb{E} \left[ Z^v \frac{\partial Z^\delta}{\partial Z^{h_i}} Z^{\delta h_{i+1}} \right]
\]

\[
= -\chi_t \sum_{i=1}^k \mathbb{E} \left[ Z^v \frac{\partial Z^\delta}{\partial Z^{h_i}} \sum_{p:p=1} Z^{\delta h_i(z_i)} \langle p, q \rangle \right]
\]

\[
= -\chi_t \sum_{i=1}^k \sum_{p:p=1} \sum_{q \geq p} \langle p, q \rangle \mathbb{E} \left[ \frac{\partial Z^\delta}{\partial Z^{h_i}} \frac{\partial Z^{x(z)}}{\partial Z^{h_i(z)}} \right]
\]

\[
= -\chi_t \hat{\mathcal{K}}(\xi_t, \tilde{\xi})
\]

It is straightforward to show that the expression for \( \hat{\mathcal{K}}(\xi_t, \tilde{\xi}) \) in Eq. (133) represents the NTK if this case.

### D.4.5. Network Specified by NETSOT \( T^+ \)

If the network is more generally represented by a NETSOT \( T^+ \) program instead of just a NETSOT \( T \) program, then our proof can be very simply modified to accommodate as follows: The new operation allowed in such a network is the production of a scalar through \textsc{moment}, say \( a = \frac{1}{n} \sum_{i=1}^n \psi(x_1^i, \ldots, x_k^i, \theta_1, \ldots, \theta^l) \). By a similar inductive argument as before, we will see that 1) \( x_i^l = x_0^l + o(1) \) for all \( i \in [k] \) and \( \theta_j^l = \theta_0^l + o(1) \) for all \( j \in [l] \), so that \( a_t = a_0 + o(1); 2) \) in the backward pass, any backpropagation through \( a \) will zero out: For example, if \( a \) is only used later in a \textsc{nonlin} \( z = \psi(y; a) \), then \( \frac{1}{\sqrt{n}} \nabla_a f = (dz, \partial_a \psi(y; a))/n \) will converge to 0 because of GIA (as \( dz \) is linear in the final layer), and the error signal at \( x^l \) times \( \sqrt{n} \) is the constant vector with entries \( \frac{1}{\sqrt{n}} \nabla_a f \), which is \( o(1) \).

Therefore, we can treat any scalar produced through \textsc{moment} as a constant fixed at initialization, and the notion of path from before carries over here without change (by assuming all nonlinearities with scalar parameters to be parameterless nonlinearities where the parameters are fixed). Then the same reasoning follows.