TRAINING INVARIANCES AND THE LOW-RANK PHENOMENON: BEYOND LINEAR NETWORKS

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ABSTRACT

The implicit bias induced by the training of neural networks has become a topic of rigorous study. In the limit of gradient flow and gradient descent with appropriate step size, it has been shown that when one trains a deep linear network with logistic or exponential loss on linearly separable data, the weights converge to rank-1 matrices. In this paper, we extend this theoretical result to the much wider class of nonlinear ReLU-activated feedforward networks containing fully-connected layers and skip connections. To the best of our knowledge, this is the first time a low-rank phenomenon is proven rigorously for these architectures, and it reflects empirical results in the literature. The proof relies on specific local training invariances, sometimes referred to as alignment, which we show to hold for a wide set of ReLU architectures. Our proof relies on a specific decomposition of the network into a multilinear function and another ReLU network whose weights are constant under a certain parameter directional convergence.

1 INTRODUCTION

Recently, great progress has been made in understanding the trajectory of gradient flow (GF) (Ji & Telgarsky, 2019; 2020; Lyu & Li, 2020), gradient descent (GD) (Ji & Telgarsky, 2019; Arora et al., 2018) and stochastic gradient descent (SGD) (Neyshabur et al., 2015; 2017) in the training of neural networks. While good theory has been developed for deep linear networks (Zhou & Liang, 2018; Arora et al., 2018), practical architectures such as ReLU fully-connected networks or ResNets are highly non-linear. This causes the underlying optimization problem (usually empirical risk minimization) to be highly non-smooth (e.g. for ReLUs) and non-convex, necessitating special tools such as the Clarke subdifferential (Clarke, 1983).

One of the many exciting results of this body of literature is that gradient-based algorithms exhibit some form of implicit regularization: the optimization algorithm prefers some stationary points to others. In particular, a wide range of implicit biases has been shown in practice (Huh et al., 2021) and proven for deep linear networks (Arora et al., 2018; Ji & Telgarsky, 2019), convolutional neural networks (Gunasekar et al., 2018) and homogeneous networks (Ji & Telgarsky, 2020). One well known result for linearly separable data is that in various practical settings, linear networks converge to the solution of the hard SVM problem, i.e., a max-margin classifier (Ji & Telgarsky, 2019), while a relaxed version is true for CNNs (Gunasekar et al., 2018). This holds even when the margin does not explicitly appear in the optimization objective - hence the name implicit regularization.

Another strong form of implicit regularization relates to the structure of weight matrices of fully connected networks. In particular, Ji & Telgarsky (2019) prove that for deep *linear* networks for binary classification, weight matrices tend to rank-1 matrices in Frobenius norm as a result of GF/GD training, and that adjacent layers' singular vectors align. The max-margin phenomenon follows as a result. In practice, Huh et al. (2021) empirically document the low rank bias across different non-linear architectures. However, their results include ReLU fully-connected networks, CNNs and ReNet, which are not all covered by the existing theory. Beyond linear fully connected networks, Du et al. (2018) show vertex-wise invariances for fully-connected ReLU networks and invariances in Frobenius norm differences between layers for CNNs. Yet, despite the evidence in (Huh et al., 2021), it has been an open theoretical question how more detailed structural relations between layers, which, e.g., imply the low-rank result, generalize to other, structured or local nonlinear and possibly non-homogeneous architectures, and how to even characterize these.

Hence, in this work, we take steps to addressing a wider set of architectures and invariances. First, we show a class of vertex and edge-wise quantities that remain invariant during gradient flow training. Applying these invariances to architectures containing fully connected, convolutional and residual blocks, arranged appropriately, we obtain invariances of the singular values in adjacent (weight) matrices. Second, we prove how the controlled singular values imply low-rank results for fully connected ReLU networks. Third, we obtain low-rank results for arbitrary non-homogeneous networks whose last few layers contain fully-connected and ResNet blocks. To the best of our knowledge, this is the first time a low-rank phenomenon is proven rigorously for these architectures.

Our theoretical results offer explanations for empirical observations on more general architectures, and apply to the experiments in (Huh et al., 2021) for ResNet and CNNs. They also include the squared loss used there, in addition to the exponential or logistic loss used in most theoretical low-rank results. Moreover, our Theorem 2 gives an explanation for the "reduced alignment" phenomenon observed by Ji & Telgarsky (2019), where in experiments on AlexNet over CIFAR-10 the ratio $\|W\|_2/\|W\|_F$ converges to a value strictly less than 1 for some fully-connected layer W towards the end of the network.

One challenge in the analysis is the non-smoothness of the networks and ensuring an "operational" chain rule. To cope with this setting, we use a specific decomposition of an arbitrary ReLU architecture into a multilinear function and a ReLU network with +1/-1 weights. This reduction holds in the *stable sign regime*, a certain convergence setting of the parameters. This regime is different from stable activations, and is implied, e.g., by directional convergence of the parameters to a vector with non-zero entries (Lemma 2). This construction may be of independent interest.

In short, we make the following contributions to analyzing implicit biases of general architectures:

- We show vertex and edge-wise weight invariances during training with gradient flow. Using these invariances, we prove that for architectures containing fully-connected layers, convolutional layers and residual blocks, when appropriately organized into matrices, adjacent matrices have the same singular value, up to initialization (Theorem 1).
- We prove that in the stable sign regime, weight matrices in a fully-connected ReLU-activated network tend to rank-1 matrices (Corollary 1). We also show a low-rank bias for arbitrary nonhomogeneous feedforward networks whose last few layers are a composition of fully-connected and ResNet blocks (Theorem 2). In particular, if the Frobenius norms of these layers diverge, then the ratio between their operator norm and Frobenius norm is bounded non-trivially by an expression C fully specified by the architecture. To the best of our knowledge, this is the first time this type of bias is shown for nonlinear, nonhomogeneous networks.
- We prove our results via a decomposition that reduces arbitrarily structured deep feedforward networks with positively-homogeneous activation (e.g., ReLU or linear) to a multilinear structure (Lemma 2).

1.1 Related works

Decomposition of fully-connected neural networks into a multilinear part and a 0-1 part has been utilized by Choromanska et al. (2015); Kawaguchi (2016) but their formulation does not apply for trajectory studies. In Section 3, we give a detailed comparison between their approach and ours. Our decomposition makes use of the construction of a tree net that has been used by Khim & Loh (2019) in analyzing generalization of fully-connected networks. We describe their approach in 2 and show how we extend their construction to arbitrary feedforward neural nets. This construction makes up the first part of the proof of our decomposition lemma. The paper also makes use of path enumeration of neural nets, which overlaps with the path-norm literature of Neyshabur et al. (2015; 2017). The distinction is that we are studying classical gradient flow, as opposed to SGD (Neyshabur et al., 2015) or its variants (Neyshabur et al., 2017).

For linear networks, low-rank bias is proven for separable data and exponential-tailed loss in Ji & Telgarsky (2019). Du et al. (2018) give certain vertex-wise invariances for fully-connected ReLU networks and Frobenius norm difference invariances for CNNs. Compared to their results, ours are slightly stronger since we prove that our invariances hold for almost every time t on the gradient flow trajectory, thus allowing for the use of a Fundamental Theorem of Calculus and downstream analysis. Moreover, the set of invariances we show is strictly larger. Radhakrishnan et al. (2020)

show negative results when generalizing the low-rank bias from (Ji & Telgarsky, 2019) to vector-valued neural networks. In our work, we only consider scalar-valued neural networks performing binary classification.

2 PRELIMINARIES AND NOTATION

For an integer $k \in \mathbb{N}$, we write the set $[k] := \{1, 2, \ldots, k\}$. For vectors, we extend the sign function $\text{sgn} : \mathbb{R} \to \{-1, 1\}$ coordinatewise as $\text{sgn} : (x_i)_{i\in[d]} \mapsto (\text{sgn}(x_i))_{i\in[d]}$. For some (usually the canonical) basis $(e_i)_{i\in[n]}$ in some vector space $\mathbb{R}^n$, for all $x \in \mathbb{R}^n$ we use the notation $[x]_i = \langle x, e_i\rangle$ to denote the i-th coordinate of x.

Clarke subdifferential, definability and nonsmooth analysis. The analysis of non-smooth functions is central to our results. For a locally Lipschitz function $f : D \to \mathbb{R}$ with open domain D, there exists a set $D^c \subseteq D$ of full Lebesgue measure on which the derivative ∇f exists everywhere by Rademacher's theorem. As a result, calculus can usually be done over the *Clarke subdifferential* defined as the set

$$\partial f(x) := \text{CONV}\left\{\lim_{i\to\infty} \nabla f(x_i) \mid x_i \in D^c, x_i \to x\right\}$$

where CONV denotes the convex hull.

The Clarke subdifferential generalizes both the smooth derivative when $f \in C^1$ (continuously differentiable) and the convex subdifferential when f is convex. However, it only admits a chain rule with an inclusion and not equality, which is though necessary for backpropagation in deep learning.

If one is willing to work with a slightly restricted set of functions - formally known as tame, Whitney stratifiable, path differentiable or definable in an o-minimal structure (Davis et al., 2020; Ji & Telgarsky, 2020; Bolte & Pauwels, 2020), the Clarke subdifferential admits an *operational* chain rule. All architectures considered in this paper are definable (Ji & Telgarsky, 2020). Here, we use the form from Ji & Telgarsky (2020).

Lemma 1 (Lemma B.9 in Ji & Telgarsky (2020))**.** *If $f : D$ open $\to \mathbb{R}$ is locally Lipschitz and defineable, then for any interval I, arc $z : I \to D$, a.e. $t \in I$, $\frac{\mathrm{d}f(z(t))}{\mathrm{d}t} = \left\langle y, \frac{\mathrm{d}z_t}{\mathrm{d}t}\right\rangle, \forall y \in \partial f(z(t))$.*

Neural networks. Consider a neural network $\nu : \mathbb{R}^d \to \mathbb{R}$. The computation graph of ν is a weighted directed graph $G = (V, E, w)$ with weight function $w : E \to \mathbb{R}$. For each neuron $v \in V$, let $\text{IN}_v := \{u \in V : uv \in E\}$ and $\text{OUT}_v := \{w \in V : vw \in E\}$ be the input and output neurons of v. Let $\{i_1, i_2, \ldots, i_d\} =: I \subset V$ and $O := \{o\} \subset V$ be the set of input and output neurons defined as $\text{IN}(i) = \emptyset = \text{OUT}(o), \forall i \in I$. Each neuron $v \in V\backslash I$ is equipped with a positively-1-homogeneous activation function σ_v (such as the ReLU $x \mapsto \max(x, 0)$, leaky ReLU $x \mapsto \max(x, \alpha x)$ for some small positive α , or the linear activation).

To avoid unnecessary brackets, we write $w_e := w(e)$ for some $e \in E$. We will also abuse notation and write $w \in \mathbb{R}^{\overline{E}}$ where $\overline{E}$ is the set of learnable weights as the vector of learnable parameters. Let P be a path in G, i.e., a set of edges in E that forms a path. We will abuse notation and write $v \in P$ for some $v \in V$ if there exists $u \in V$ such that $uv \in P$ or $vu \in P$. Let ρ be the number of distinct paths from any $i \in I$ to $o \in O$. Let $\mathcal{P} := \left\{p_1, \ldots, p_\rho\right\}$ be the enumeration of these paths. For a path $p \in \mathcal{P}$ and an input x to the neural net, denote x_p the coordinate of x used in p.

Given a binary classification dataset $\left\{(x_i, y_i)\right\}_{i\in[n]}$ with $x_i \in \mathbb{R}^d, \|x_i\| \leq 1$ and $y_i \in \{-1, 1\}$, we minimize the empirical risk $\mathcal{R}(w) = \frac{1}{n}\sum_{i=1}^n \ell(y_i\nu(x_i)) = \frac{1}{n}\sum_{i=1}^n \ell(\nu(y_ix_i))$ with loss $\ell : \mathbb{R} \to \mathbb{R}$, using gradient flow $\frac{\mathrm{d}w(t)}{\mathrm{d}t} \in -\partial\mathcal{R}(w(t))$.

As we detail the architectures used in this paper, we recall that the activation of each neuron is still positively-homogeneous. The networks considered here are assumed to be bias-free unless stated otherwise.

Definition 1 (Feedforward networks)**.** *A neural net ν with graph G is a* feedforward network *if G is a directed acyclic graph (DAG).*

Definition 2 (Fully-connected networks)**.** *A feedforward network ν with graph G is a* fully-connected network *if there exists partition of V into $V = (I \equiv V_1) \sqcup V_2 \sqcup \ldots \sqcup (V_{L+1} \equiv O)$ such that for all $u, v \in V, uv \in E$ iff there exists $i \in [L]$ such that $u \in V_i$ and $v \in V_{i+1}$.*

Definition 3 (Tree networks)**.** *A feedforward network ν with graph G is a* tree network *if the underlying undirected graph of G is a tree (undirected acyclic graph).*

Examples of feedforwards networks include ResNet (He et al., 2016), DenseNet (Huang et al., 2017), CNNs (Fukushima, 1980; LeCun et al., 2015) and other fully-connected ReLU architectures.

For a fully-connected network ν with layer partition $V =: V_1 \sqcup \ldots \sqcup V_{L+1}$ where L is the number of (hidden) layers, let $n_i := |V_i|$ be the number of neurons in the i-th layer and enumerate $V_i = \{v_{i,j}\}_{j\in[n_i]}$. Weights in this architecture can be organized into matrices $W^{[1]}, W^{[2]}, \ldots, W^{[L]}$ where $\mathbb{R}^{n_{i+1}\times n_i} \ni W^{[i]} = ((w_{v_{i,j}v_{i+1,k}}))_{j\in[n_i],k\in[n_{i+1}]}$, for all $i \in [L]$.

Tree networks. Most practical architectures are not tree networks, but they have been used to prove generalization bounds for adversarial risks. In particular, for fully-connected neural networks f whose activations are monotonically increasing and 1-Lipschitz, Khim & Loh (2019) defined the *tree transform* as the tree network $Tf(x; w) = \sum_{p_L=1}^{n_L} W^{[L]}_{1,p_L} \sigma\left(\ldots \sum_{p_2=1}^{n_2} W^{[2]}_{p_3,p_2} \sigma\left(w_{p_2..p_L} + \sum_{p_1=1}^{n_1} W^{[1]}_{p_2,p_1} x_{p_1}\right)\right)$ for vectors w with $\prod_{j=2}^{L} n_j$ entries, indexed by an L-tuple $(p_2, \ldots, p_L)$. We extend this idea in the next section.

3 Structural lemma: decomposition of deep network

We begin with a decomposition of a neural network into a multilinear and a non-weighted nonlinear part, which will greatly facilitate the chain rule that we need to apply in the analysis. Before stating the decomposition, we need the following definition of a path enumeration function, which computes the product of all weights and inputs on each path of a neural network.

Definition 4 (Path enumeration function)**.** *Let ν be a feedforward neural network with graph G and paths $\mathcal{P} = \{p_1, \ldots, p_\rho\}$. The path enumeration function h is defined for this network as $h : (x_1, x_2, \ldots, x_d) \mapsto \left(x_p \prod_{e\in p} w_e\right)_{p\in\mathcal{P}}$ where $x_p := x_k$ such that $i_k \in p$.*

We first state the main result of this section, proven in Appendix B.

Lemma 2 (Decomposition)**.** *Let $\nu : \mathbb{R}^d \to \mathbb{R}$ be a feedforward network with computation graph G, and ρ is the number of distinct maximal path in G. Then there exists a tree network $\mu : \mathbb{R}^\rho \to \mathbb{R}$ such that $\nu = \mu \circ h$ where $h : \mathbb{R}^d \to \mathbb{R}^\rho$ is the path enumeration function of G. Furthermore, all weights in μ are either -1 or $+1$ and fully determined by the signs of the weights in ν.*

Path activation of ReLU networks in the literature. The viewpoint that for every feedforward network ν there exists a tree network μ such that $\nu = \mu \circ h$ is not new and our emphasis here is on the fact that the description of $\mu : \mathbb{R}^\rho \to \mathbb{R}$ is fully determined by the signs of the weights. Indeed, in analyses of the loss landscape (Choromanska et al., 2015; Kawaguchi, 2016), ReLU networks are described as a sum over paths:

$$\nu(x; w) = \sum_{p\in\mathcal{P}} Z_p(x; w) \prod_{e\in p} w_e = \left\langle (Z_p(x; w))_{p\in\mathcal{P}}, h(x; w)\right\rangle_{\mathbb{R}^\rho}, \tag{1}$$

where $Z_p(x; w) = 1$ iff all ReLUs on path p are active (have nonnegative preactivation) and 0 otherwise. One can then take μ as a tree network with no hidden layer, ρ input neurons all connected to a single output neuron. However, this formulation complicates analyses of gradient trajectories, because of the explicit dependence of Z_p on numerical values of w. In our lemma, μ is a tree network whose description depends only on the signs of the weights. If the weight signs (not necessarily the ReLU activation pattern!) are constant, μ is fixed, allowing for a chain rule to differentiate through it. That weight signs are constant is realistic, in the sense that it is implied by directional parameter convergence (Section 4.1). To see this, compare the partial derivative with respect to some w_e (when it exists) between the two approaches, in the limit where weight signs are constant

$$\text{(using Lemma 2)} \qquad \partial\nu/\partial w_e = \sum_{p\in\mathcal{P}|e\in p} [\nabla_w \mu(x; w)]_p \cdot x_p \prod_{f\in p, f\neq e} w_f, \tag{2}$$

$$\text{(using } Z_p \text{ in Eqn 1)} \qquad \partial\nu/\partial w_e = \sum_{p\in\mathcal{P}|e\in p} \left(w_e \partial Z_p(x; w)/\partial w_e + Z_p(x; w)\right) \prod_{f\in p, f\neq e} w_f. \tag{3}$$

In particular, the dependence of Equation 2 on w_e is extremely simple. This usefulness of this fact will be made precise in the next section when we study invariances.

Proof sketch. The proof contains two main steps. First, we 'unroll' the feedforward network into a tree network that computes the same function by adding extra vertices, edges and enable weight sharing. This step is part of the tree transform in Khim & Loh (2019) if the neural network is a fully-connected network; we generalize it to work with arbitrary feedforward networks. Second, we "pull back" the weights towards the input nodes using positive homogeneity of the activations: $a \cdot \sigma(x) = \text{sgn}(a) \cdot \sigma(x|a|)$. This operation is done on vertices closest (in number of edges on the unique path between any two vertices in a tree) to the output vertex first and continue until all vertices have been processed. Finally, all the residual signs can be subsumed into μ by subdividing edges incident to input neurons. We give a quick illustration of the two steps described above for a fully-connected ReLU-activated network with 1 hidden layer in the Appendix A.

4 Main Theorem: Training invariances

In this section, we put the previous decomposition lemma to use in proving an implicit regularization property of gradient flow in training deep neural networks.

4.1 Stable sign regime: a consequence of directional convergence

Recall the gradient flow curve $\{w(t)\}_{t\in[0,\infty)}$ defined by the differential inclusion $\frac{\mathrm{d}w(t)}{\mathrm{d}t} \in -\partial\mathcal{R}(w(t))$. We first state the main assumption in this section.

Assumption 1 (Stable sign regime)**.** *For some $t_0 < t_N \in [0,\infty]$, we assume that for all $t \in [t_0, t_N)$, $\text{sgn}(w(t)) = \text{sgn}(w(t_0))$. If this holds, we say that gradient flow is in a* stable sign regime. *Without loss of generality, when using this assumption, we identify t_0 with 0 and write "for some $t \geq 0$" to mean "for some $t \in [t_0, t_N)$".*

In fact, the following assumption - the existence and finiteness part of which has been proven in (Ji & Telgarsky, 2020) for homogeneous networks, is sufficient.

Assumption 2 (Directional convergence to non-vanishing limit in each entry)**.** *We assume that $\frac{w(t)}{\|w(t)\|_2} \xrightarrow{t\to\infty} \overline{w}$ exists, is finite in each entry and furthermore, for all $e \in E, \overline{w}_e \neq 0$.*

Motivation and justification. It is straightforward to see that Assumption 1 follows from Assumption 2 but we provide a proof in the Appendix (Claim 1). Directional convergence was proven by Ji & Telgarsky (2020) using the exponential/logistic loss for the class of homogeneous networks, under additional mild assumptions. This fact justifies the first part of Assumption 2 for these architectures. The second part of Assumption 2 is pathological for our case, in the sense that directional convergence alone does not imply stable signs (for example, a weight that converges to 0 can change sign an infinite number of times).

Pointwise convergence is too strong in general. Note also that assuming pointwise convergence of the weights (i.e. $\lim_{t\to\infty} w(t)$ exists and is finite) is a much stronger statement, which is not true for the case of exponential/logistic loss and homogeneous networks (since $\|w(t)\|_2$ diverges, see for example Lyu & Li (2020), Ji & Telgarsky (2020), Ji & Telgarsky (2019)). Even when pointwise convergence holds, it would immediately reduce statements on asymptotic properties of gradient flow on ReLU activated architectures to that of linearly activated architectures. One may want to assume that gradient flow starts in the final affine piece prior to its pointwise convergence and thus activation patterns are fixed throughout training and teh behavior (multi)linear. In contrast, directional convergence of the weights *does not* imply such reduction from the ReLU-activation to the linear case (since, for example, linear pieces of ReLU networks are not necessarily convex (Hanin & Rolnick, 2019) or see a counter-example in Claim 2).

Stable sign implication. The motivation for Assumption 1 is the fact that weights in the tree network μ in the statement of Lemma 2 are fully determined by the *signs* of the weights in the original feedforward network ν. Thus, under Assumption 1, one can completely fix the weights of μ - it has no learnable parameters. Since we have the decomposition $\nu = \mu \circ h$ where h is the

path enumeration function, dynamics of μ are fully determined by dynamics of h in the stable sign regime. To complete the picture, observe that h is highly multilinear in structure: the degree of a particular edge weight w_e in each entry of h is at most 1 for all edge e by definition of a path; and if ν is fully-connected, then h is a tensor in $\mathbb{R}^{n_1 \times n_2 \times \ldots \times n_L}$.

4.2 Training invariances

First, we state an assumption on the loss function, which holds for most losses used in practice, such as the logistic loss, exponential loss or squared loss.

Assumption 3 (Differentiable loss)**.** *The loss function $\ell : \mathbb{R} \to \mathbb{R}$ is differentiable everywhere.*

Lemma 3 (Vertex-wise invariance)**.** *Under Assumption 1, and 3, for all $v \in V \backslash \{I \cup O\}$ such that all edges incident to v have learnable weights, for a.e. time $t \geq 0$,*

$$\sum_{u \in \text{IN}_v} w_{uv}^2(t) - \sum_{b \in \text{OUT}_v} w_{vb}^2(t) = \sum_{u \in \text{IN}_v} w_{uv}^2(0) - \sum_{b \in \text{OUT}_v} w_{vb}^2(0). \tag{4}$$

If we also have $\text{IN}_u = \text{IN}_v = \text{IN}$ and $\text{OUT}_u = \text{OUT}_v = \text{OUT}$ then for a.e. time $t \geq 0$,

$$\sum_{a \in \text{IN}} w_{au}(t) w_{av}(t) - \sum_{b \in \text{OUT}} w_{ub}(t) w_{vb}(t) = \sum_{a \in \text{IN}} w_{au}(0) w_{av}(0) - \sum_{b \in \text{OUT}} w_{ub}(0) w_{vb}(0). \tag{5}$$

Comparison to Du et al. (2018) A closely related form of Equation 4 in Lemma 3 has appeared in Du et al. (2018) (Theorem 2.1) for fully-connected ReLU/leaky-ReLU networks. In particular, the authors showed that the rate of change of difference between incoming and outgoing weights is 0. Invoking the Fundamental Theorem of Calculus (FTC) over this statement will return ours. However, their proof may not hold over a nonnegligible set of time t due to the use of the operational chain rule (Lemma 1) that holds only for almost all w_e. Thus the FTC can fail. The stronger form we showed here is useful in proving downstream algorithmic consequences, such as the low rank phenomenon. Furthermore, our result also holds for arbitrary feedforward architectures and not just the fully-connected case.

Before we put Lemma 3 to use, we list definitions of some ResNet variants.

Definition 5. *Denote ResNetIdentity, ResNetDiagonal and ResNetFree to be the version of ResNet described in He et al. (2016) where the residual block is defined respectively as*

1. *$r(x; U, Y) = \sigma(U\sigma(Yx) + Ix)$ where $x \in \mathbb{R}^a, Y, U^\top \in \mathbb{R}^{b \times a}$, and I is the identity,*
2. *$r(x; U, Y, D) = \sigma(U\sigma(Yx) + Dx)$ where $x \in \mathbb{R}^a, Y, U^\top \in \mathbb{R}^{b \times a}$, and D is diagonal,*
3. *$r(x; U, Y, Z) = \sigma(U\sigma(Yx) + Zx)$ where $x \in \mathbb{R}^a, Y \in \mathbb{R}^{b \times a}, U \in \mathbb{R}^{c \times b}$ and $Z \in \mathbb{R}^{c \times a}$.*

ResNetIdentity is the most common version of ResNet used in practice and is described in Equation 1 of (He et al., 2016). ResNetFree is described in Equation 2 of (He et al., 2016) but is less commonly used. Note that although ResNetIdentity is a special case of ResNetDiagonal, which is in turn a special case of ResNetFree. However, theorems for ResNetFree, for example, do not generalize trivially to the remaining variants, due to the restriction of Lemma 3 and Lemma 4 to vertices adjacent to all learnable weights and layers containing all learnable weights.

When applying Lemma 3 to specific architectures, we obtain the following:

Theorem 1 (Matrix-wise invariances)**.** *Recall that a convolutional layer with number of input kernels a, kernel size b and number of output kernels c and is a tensor in $\mathbb{R}^{a \times b \times c}$. Under Assumptions 1 and 3, we have the following matrix-wise invariance for a.e. time $t \geq 0$:*

$$W_2(t)^\top W_2(t) - W_1(t) W_1(t)^\top = W_2(0)^\top W_2(0) - W_1(0) W_1(0)^\top \tag{6}$$

for:

1. *(Fully-connected layers) $W_1 \in \mathbb{R}^{b \times a}$ and $W_2 \in \mathbb{R}^{c \times b}$ consecutive fully-connected layers,*
2. *(Convolutional layers) W_1 is convolutional, viewed as a flattening to a matrix $\mathbb{R}^{c \times (a \times b)}$, and W_2 adjacent convolutional, viewed as a flattening to a matrix $\mathbb{R}^{(d \times e) \times c}$,*

3. *(Within residual block of ResNet)* $W_1 = Y$ *and* $W_2 = U$ *where* $r(x; U, Y, Z)$ *is a residual block of ResNetIdentity, ResNetDiagonal or ResNetFree,*

4. *(Between residual blocks of ResNet)* $W_1 = \begin{bmatrix} U_1 & Z_1 \end{bmatrix}$, $W_2 = \begin{bmatrix} Y_2 \\ Z_2 \end{bmatrix}$ *where* $r(x; U_j, Y_j, Z_j)$, $j \in \{1, 2\}$ *are consecutive ResNetFree blocks,*

5. *(Convolutional-fully-connected layers)* W_1 *convolutional, viewed as a flattening to a matrix* $\mathbb{R}^{c \times (a \times b)}$ *and* W_2 *adjacent fully-connected layer, viewed as an rearrangement to* $\mathbb{R}^{d \times c}$*,*

6. *(Convolutional-ResNetFree block)* W_1 *convolutional, viewed as a flattening to a matrix* $\mathbb{R}^{c \times (a \times b)}$ *and* W_2 *is a rearrangement of* $\begin{bmatrix} U & Z \end{bmatrix}$ *into an element of* $\mathbb{R}^{d \times c}$*, where* $r(x; U, Y, Z)$ *is an adjacent ResNetFree block,*

7. *(ResNetFree block-fully-connected layers and vice versa)* $W_1 = \begin{bmatrix} U & Z \end{bmatrix} \in \mathbb{R}^{b \times a}$ *and* $W_2 \in \mathbb{R}^{c \times b}$ *adjacent fully-connected or* $W_1 \in \mathbb{R}^{b \times a}$ *fully-connected and* $W_2 = \begin{bmatrix} Y \\ Z \end{bmatrix} \in \mathbb{R}^{c \times b}$ *adjacent ResNet block where* $r(x; U, Y, Z)$ *is the ResNetFree block.*

We emphasize that the above theorem only makes *local* requirements on the neural network, to have local parts that are either fully-connected, convolutional or a residual block. The only global architecture requirement is feedforward-ness. The first point of Theorem 1 admits an extremely simple proof for the linear fully-connected network case in Arora et al. (2018) (Theorem 1) but has not been generalized to other architectures.

Significance of Theorem 1. Assume for simplicity that the right hand side in Equation 6 is 0, then the singular values of W_1 and W_2 are the same for each of the cases listed in Theorem 1. If we can form a chain of matrices whose singular values are the same by iteratively invoking Theorem 1 then all matrices considered have the same singular values as the final fully-connected layer that connects to the output. Recall that our networks are scalar-valued, so the final layer is a row vector, which is rank 1 and thus all layers considered in the chain have rank 1, which is useful in the next section.

Proof sketch of Theorem 1. Given Lemma 3, we demonstrate the proof for the first point. The remaining points admit the exact same proof technique but on different matrices, which can get messy and require some bookkeeping. Let $W_1 \in \mathbb{R}^{b,a}$ and $W_2 \in \mathbb{R}^{c,b}$ be two consecutive fully-connected layers for some $a, b, c \in \mathbb{N}$ number of vertices in these layers. Apply Equation 4 of Lemma 3 to each of the b shared neurons between these two layers, one get the diagonal entries of Equation 6 of the Theorem. Now, apply Equation 5 to each pair among the b shared neurons between these two layers, one get the off-diagonal entries of Equation 6.

We give a definition of layer for architectures where weights are not necessarily organized into matrices - say ResNet or DenseNet.

Definition 6 (Layer)**.** *Let* $F \subset E$ *be such that 1) for all* $e \neq f \in F$*, there is no path that contains both* e *and* f*; and 2) the graph* $(V, E \backslash F, w)$ *is disconnected. Then* F *is called a* layer *of* G*.*

For this definition, we have the following invariance:

Lemma 4 (Edge-wise invariance)**.** *Under Assumption 1, and 3, for all layers* F *and* F' *that contains all learnable weights, for a.e. time* $t \geq 0$*,*

$$\sum_{e \in F} w_e^2 - \sum_{f \in F'} w_f^2 = \sum_{e \in F} w_e^2(0) - \sum_{f \in F'} w_f^2(0). \tag{7}$$

Since IN_o *forms a layer, we also have*

$$\sum_{e \in F} w_e^2 - \sum_{v \in \text{IN}_o} w_{vo}^2 = \sum_{e \in F} w_e^2(0) - \sum_{v \in \text{IN}_o} w_{vo}^2(0). \tag{8}$$

Significance of Lemma 4. A flattening of a convolutional parameter tensor and a stacking of matrices in a ResNetDiagonal and ResNetFree block forms a layer. This lemma implies that the squared Frobenius norm of these matrices in the same network differs by a value that is fixed at

initialization. This lemma also gives a direct implicit regularization for networks with biases, by treating neurons with bias as having an extra in-edge whose weight is the bias, from an extra in-vertex which is an input vertex with fixed input value 1.

4.3 Proof sketch of Lemma 3 and Lemma 4

All proofs in Lemma 3, Lemma 4 and Theorem 1 share the same technique of double counting paths, which we explain next. For simplicity, let us here assume that we are working with a network that is differentiable everywhere in some domain that we are considering – we give a full general proof in the Appendix. The main proof idea has been used in (Arora et al., 2018) and involves simply writing down the partial derivative of the risk. We have for some particular weight $w_e, e \in E$, via the smooth chain rule

$$\frac{\partial \mathcal{R}(w)}{\partial w_e} = \frac{1}{n}\sum_{i=1}^{n} l'(y_i \nu(x_i; w)) \cdot y_i \cdot \frac{\partial \nu(w)}{\partial w_e} \tag{9}$$

$$= \frac{1}{n}\sum_{i=1}^{n} l'(y_i \nu(x_i; w)) \cdot y_i \cdot \sum_{p \in \mathcal{P}, p \ni e} \left[\mu'(x_i; w)\right]_p \cdot (x_i)_p \prod_{f \in p, f \neq e} w_f \tag{10}$$

where in the second line, we invoke the decomposition Lemma 2 and emphasize that μ has no learnable parameters in the stable sign regime. Now multiply w_e to the above expression to get

$$w_e \frac{\partial \mathcal{R}(w)}{\partial w_e} = \sum_{p \in \mathcal{P}, p \ni e} \frac{1}{n}\sum_{i=1}^{n} A_{i,p}(w) \tag{11}$$

where $A_{i,p}(w) = l'(y_i \nu(x_i; w)) \cdot y_i \cdot \left[\mu'(x_i; w)\right]_p \cdot (x_i)_p \prod_{f \in p} |w_f|$. Notice that $A_{i,p}(w)$ does not depend explicitly on the edge e we are taking the partial derivative over (only through w). Thus, we can sum over in-edges and out-edges of a particular v satisfying the assumption of Lemma 3 to get

$$\sum_{u \in \mathrm{IN}_v} w_{uv} \frac{\partial \mathcal{R}(w)}{\partial w_{uv}} = \sum_{p \in \mathcal{P}, p \ni v} \frac{1}{n}\sum_{i=1}^{n} A_{i,p}(w) = \sum_{b \in \mathrm{OUT}_v} w_{vb} \frac{\partial \mathcal{R}(w)}{\partial w_{vb}}. \tag{12}$$

Note that the only difference between Equations 11 and 12 is the set of paths that it is summing over, and we double count this set of paths.

We use the definition of gradient flow to get $\partial \mathcal{R}(w)/\partial w_e = \mathrm{d}w_e(t)/\mathrm{d}t$ and integrate with respect to time using a FTC to get the first part of Lemma 3. To get the second part of Lemma 3, we double count the set of jagged paths defined as all paths from I to v together with all paths from u to O and vice versa. Finally, to get Lemma 4, we double count the set of all paths $\mathcal{P}$.

5 Consequences: Low rank phenomenon for nonlinear nonhomogeneous deep feedforward net

We apply the results from previous parts to prove a low-rank bias result for a large class of feedforward networks. To the best of our knowledge, this is the first time such a result is shown for this class of deep networks, although the linear network analog has been known for some time.

In light of Theorem 1, we have a definition of matrix representations of a layer:

Definition 7 (Matrix representation of a layer)**.** *The matrix representation for a ResNetFree block $r(x; U, Y, Z)$ is $\begin{bmatrix} U & Z \end{bmatrix}$; for a $T^{a,b,c} \in \mathbb{R}^{a,b,c}$ convolutional tensor is the flattening to an element of $\mathbb{R}^{a \times (b \times c)}$; and for a fully-connected layer is the weight matrix itself.*

Theorem 2 (Reduced alignment for non-homogeneous networks)**.** *Under Assumption 1 and 3, let ν consist of an arbitrary feedforward neural network η, followed by $K \geq 0$ convolutional layers $(T^{a_k,b_k,c_k})_{k \in [K]}$, followed by $M \geq 0$ layers that are either ResNetFree blocks or fully-connected layers; and finally ending with a linear fully-connected layer Fin. For $j \in [K+M]$, denote $W^{[j]}$ the matrix representation of the j-th layer after η, $N_r(j)$ the number of ResNetFree blocks between*

j and Fin exclusively and $V_c(j) := \max \dim W^{[M+1]} \cdot \prod_{j<k\leq M} \min(a_k, b_k)$ if $j \leq M$ and 1 otherwise. Then there exists a constant $D \geq 0$ fixed at initialization such that for a.e. time $t > 0$,

$$\frac{1}{8^{N_r(j)} V_c(j)} \|W^{[j]}(t)\|_F^2 - \|W^{[j]}(t)\|_2^2 \leq D, \ \forall j \in [K+M]. \tag{13}$$

Furthermore, assume that $\|W^{[j]}\|_F \to \infty$ for some $j \in [K+M]$, then we have, in the limit of $t \to \infty$:

$$1/\min\left(\textit{rank}(W^{[k]}), 8^{N_r(j)} V_c(j)\right) \leq \|W^{[k]}(t)\|_2^2 / \|W^{[k]}(t)\|_F^2 \leq 1, \tag{14}$$

where rank returns the number of nonzero singular value of a matrix. In particular, for the last few fully-connected layers j with $N_r(j) = 0$ and $V_c(j) = 1$, we have, in the limit of $t \to \infty$:

$$\left\| \frac{W^{[j]}(t)}{\|W^{[j]}(t)\|_F} - u_j(t) v_j^\top(t) \right\|_F \xrightarrow{t\to\infty} 0, \forall k \in [M], \qquad |\left\langle v_{j+1}, u_j \right\rangle| \xrightarrow{t\to\infty} 1, \tag{15}$$

where u_j and v_j is the left and right principal singular vector of $W^{[j]}$.

Corollary 1. *For fully-connected networks with ReLU activations, trained with linearly separable data under logistic loss ℓ, under the assumptions that $\mathcal{R}(w(0)) < \ell(0)$ and the limiting direction of weight vector (which exists (Ji & Telgarsky, 2020)) has no 0 entries, Equation 15 holds.*

Significance Equation 13 and its limiting counterpart Equation 14 quantifies a low-rank phenomenon by providing a lower bound on the ratio of the largest squared singular value (the operator norm) to the sum of all squared singular values (the Frobenius norm). This lower bound depends on the *number* (not dimensions) of ResNetFree layers (N_r) and *certain dimensions* of convolutional layers (V_c). When the dimensions of ResNetFree layers are large, $\max \dim W^{[M+1]}$ is small and number of input channels of convolutional layers are large, this lower bound is strictly better than the trivial lower bound of $1/\text{rank}(W^{[k]})$. This is a quantification of the *reduced alignment* observed in (Ji & Telgarsky, 2019). In particular, for the last few fully connected layers (Equation 15, Corollary 1), the lower bound matches the upper bound of 1 in the limit of Frobenius norm tending to infinity and the limiting weight matrices have rank 1 and adjacent layers align.

5.1 Proof sketch

The proof is similar to that of Lemma 2.6 in (Ji & Telgarsky, 2019). Fix a $j \in [M+1]$ and invoke Lemma 4 over the layer $W^{[j]}$ to get $\|W^{[j]}\|_F^2 - \|Fin\|_F^2 = D_1$ for some D_1 fixed at initialization. But since our network is scalar-valued, Fin is a vector and thus $\|Fin\|_F^2 = \|Fin\|_2^2$. Now invoking Theorem 1 for consecutive pairs of layers, we can prove that $\|W^{[k]}\|_2^2 \geq C\|W^{[k+1]}\|_2^2 - D_{2,k}$ for $C = 1/8$ if the $k+1$ layer is a ResNetFree block (Lemma 10), $C = 1/\min(a_{k+1}, b_{k+1})$ if the $k+1$ layer is a convolutional layer, $C = \max \dim W^{[M+1]}$ if $k = M$ (Lemma 9) and $C = 1$ otherwise, for some $D_{2,k}$ fixed at initialization, for all k from j to $M+K$. Telescope and subtract from $\|W^{[j]}\|_F^2$ to get the final result. The rest follows from Lemma 2.6 in (Ji & Telgarsky, 2019).

6 Concluding remarks and Future directions

In this paper, we extend the proof of the low rank phenomenon, which has been widely observed in practice, beyond the linear network case. In particular, we address a variety of nonlinear architectural structures, homogeneous and non-homogeneous, which in this context have not been addressed theoretically before. To this end, we decomposed a feedforward ReLU/linear activated network into a composition of a multilinear function with a tree net. If the weights converge in direction to a vector with non-zero entries, the tree net is eventually fixed, allowing for chain rules to differentiate through. This leads to various matrix-wise invariances between fully-connected, convolution layers and ResNet blocks, enabling us to control the singular values of consecutive layers. In the end, we obtain a low-rank theorem for said local architectures.

Proving convergence to stable sign regime for wider architectures will strengthen Theorem 2. Another direction is to connect our low-rank bias results to the max-margin implicit regularization literature, which has been shown for linear networks and, more recently, certain 2-homogeneous architecture (Ji & Telgarsky, 2020). Another direction is to extend alignment results to vector-valued neural nets, where Radhakrishnan et al. (2020) gave a certain negative results.

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A Illustration of Lemma 2

We give a quick illustration of the two steps described in Section 3 for a fully-connected ReLU-activated network with 1 hidden layer. Figure 1 describes the unrolling of the neural network (Figure 1a) into a tree network (Figure 1b). Figure 2a describes the weight pull-back in the hidden layer and Figure 2b describes the weight pull-back in the input layer. It is clear that the inputs of the tree net in Figure 2b are coordinates of the path enumeration function $h(x; w)$ in this example. Furthermore, weights in the tree net depend entirely on the signs of the original weights. The rest of the proof argues this intuition for general feed-forward neural nets. As a remark, in general, ρ is a very large number - exponential in the number of layers for a fully-connected net with fixed width.

B Proof of Lemma 2

We first prove an absolute-valued version of Lemma 2 and show that the extension to Lemma 2 is straightforward. In other words, we first prove

Lemma 5 (Absolute-valued decomposition)**.** *For an arbitrary feed-forward neural network $\nu : \mathbb{R}^d \to \mathbb{R}$, there exists a tree network $\mu' : \mathbb{R}^\rho \to \mathbb{R}$ such that $\nu = \mu' \circ h'$ where h' is the absolute-valued path enumeration function defined as $h'(x) = \left(x_p \prod_{e \in p} |w_e|\right)_{p \in \mathcal{P}}$. Furthermore, the weights of μ' is in $\{-1, 1\}$ and only depends on the sign of the weights of the original network ν.*

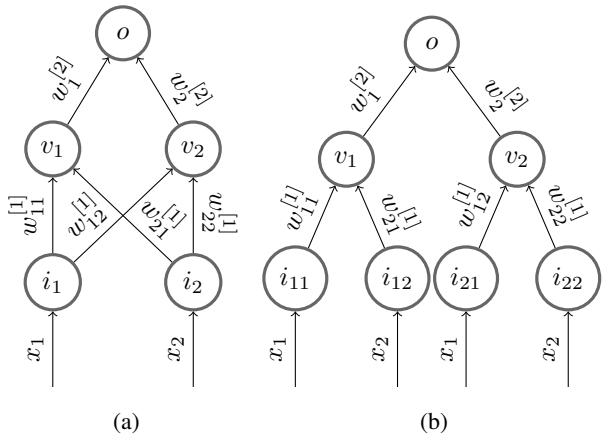

Figure 1: Transformation of a feedforward network into a tree net. All nodes apart from the input nodes use ReLU activation. The two neural nets drawn here compute the same function. This idea has been used in Khim & Loh (2019) to prove generalization bounds for adversarial risk.
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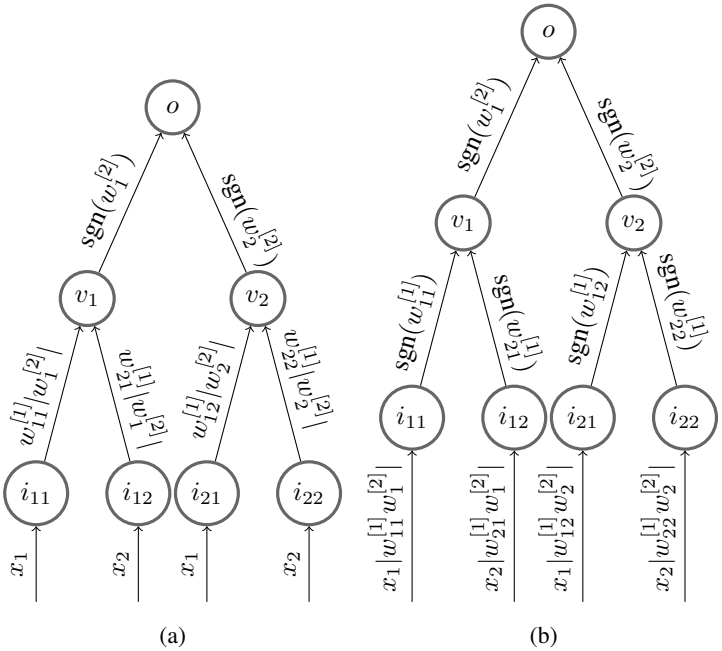


Figure 2: Pulling back of weights in a tree net. All nodes apart from the input nodes use the ReLU activation. The original net was drawn in Figure 1a and 1b. This is possible due to the positive-homogeneity of the activation function. From Figure 2b, one can recover the final tree net in Theorem 2 with weights from $\{-1, +1\}$ and input from the path enumeration function h of the neural net by subdividing the edge incident to the input neurons and assign weights corresponding to $\mathrm{sgn}(h(x))$.

We first give some extra notation for this section. In general, we define:

- $\wp(S)$ to be the finite power set of some finite set S.
- $|p| \in \mathbb{N}_{\geq 0}$ to be the cardinality of a set p. When p is a path then it is viewed as the number of edges.

To make it clear which graph we are referring to, define for an arbitrary feedforward neural network $\nu : \mathbb{R}^d \to \mathbb{R}$ with computation graph $G = (G[V], G[E], G[w])$:

- $I_G = \{i_1^G, \ldots, i_d^G\}$ to be the set of input node of G and $O_G = \{o_G\}$ to be the set of the single output node of G.
- $\mathcal{P}_G$ to be the enumeration of all paths from any input node in I_G to the output node o_G.
- $\mathcal{H}_G$ to be the enumeration of all paths from *any* node $v \in G[V]$ to the output node o_G. Note that if G has more than 2 vertices then $\mathcal{H}_G \supset \mathcal{P}_G$.
- Each $v \in G[V]$ to be equipped with a fix activation σ_v that is positively-1-homogeneous. To be precise, G is enforced to be a DAG, is connected and is simple (no self-loop, at most 1 edge between any pair of vertices). Each node v of $G[V]$ is equipped with: an activation function $G[\sigma](v)$ that is positively-1-homogeneous; a pre-activation function defined as:

$$(G[\text{PRE}](v))(x) = \begin{cases} x_j & \text{if } v \equiv i_j^G \text{ for some } j \in [d] \\ \sum_{u \in \text{IN}_v} \text{POST}_v(x) w_{uv} & \text{otherwise;} \end{cases} \tag{16}$$

  and a post-activation function defined as

$$(G[\text{POST}](v))(x) = \sigma_v((G[\text{PRE}](v))(x)) \tag{17}$$

  Note that $\text{POST}_{o_G} = \nu$.
- v_p^G, e_p^G to be the vertex and edge, respectively, furthest from o_G on some path p of G.
- x_p^G to be the unique x_j such that $i_j^G \in p$.

Definition 8 (Hasse diagram of inclusion)**.** *Let S be a finite set and a set $\mathcal{S} \subset \wp(S)$ of elements in S. A* Hasse diagram *of $\mathcal{S}$ is a directed unweighted graph* $\text{HASSE}(\mathcal{S}) = (\mathcal{S}, E)$ *where for any $p, q \in \mathcal{S}$, $pq \in E$ iff $p \subseteq q$ and $|q| - |p| = 1$.*

Definition 9 (Unrolling of feedforward neural networks)**.** *The* unrolled tree neural network *τ_G of G is a tree neural network with computation graph T_G where*

- *Unweighted graph $(T_G[V], T_G[E]) = \text{HASSE}(\mathcal{H}_G)$. In particular $T_G[V] = \mathcal{H}_G$ and we identify vertices of T_G with paths in G.*
- *Weight function $T_G[w] : T_G[E] \ni pq \mapsto G[w](e_p)$.*
- *Activation $T_G[\sigma](v) := G[\sigma](v_p)$.*

Lemma 6 (Unrolled network computes the same function)**.** *Fix an arbitrary feedforward neural network $\nu : \mathbb{R}^d \to \mathbb{R}$ with computation graph G. Let τ_G be the unrolled tree network of G with computation graph T_G. Then $\nu = \tau_G$.*

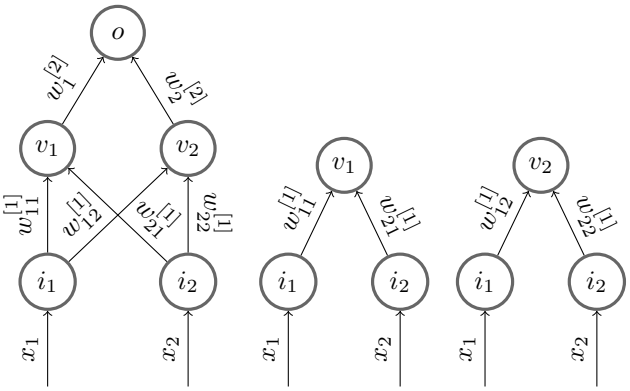
Proof. We proceed with induction on $\alpha_G := \max_{p \in \mathcal{P}} |p|$ the longest path between any input node and the output node of G. In the base case, set $\alpha_G = 0$. Then $V_G = \{o_G\}$ is a singleton and the neural network ν computes the activation of the input and return it. $\mathcal{H}_G = V_T = \{p_0\}$ then is a singleton containing just the trivial path that has just the output vertex of G and no edges. The activation function attached to p_0 in T, by construction, is the activation of o_G. Thus, τ also simply returns the activation of the input.

Assume that $\tau_G = \nu$ for any ν with graph G such that $\alpha_G \leq t - 1$ for some $t \geq 1$; and for the τ constructed as described. We will show that the proposition is also true when ν has graph G with $\alpha_G = t$. Fix such a ν and G that $\alpha_G = t$. We prove this induction step by:

1. First constructing G' from G such that $\nu' = \nu$ where ν' is the neural network computed by G'.
2. Then showing that $T_G = G'$ by constructing an isomorphism $\pi : G'[V] \to T_G[V]$ that preserves E, w and σ.

The construction of G' An illustration of the following steps can be found in Figure 3. Recall that $\text{IN}_{o_G} = \{v_1, \ldots, v_m\}$ is the set of in-vertices of o_G.

1. Create m distinct, identical copies of G: $G_1, \ldots, G_m$.
2. For each $j \in [m]$, remove from G_j all vertices u (and their adjacent edges) such that there are no directed path from u to v_j.
3. We now note that $\alpha_{G_j} \leq t - 1$ (to be argued) and invoke inductive hypothesis over G_j to get an unrolled tree network τ_j with graph T_j such that $\tau_j = \nu_j$ where ν_j is the neural network computed by G_j.
4. Finally, construct G' by creating a new output vertex $o_{G'}$ and connect it to the output vertices o_{T_j} for all $j \in [m]$. As a sanity check, since each T_j is a tree network, so is G'. More precisely,
   (a) $G'[V] = \{o_{G'}\} \cup \bigcup_{j=1}^{m} T_j[V]$;
   (b) $G'[E] = \{o_{G_j} o_{G'} \mid j \in [m]\} \cup \bigcup_{j=1}^{m} T_j[E]$
   (c) $G'[w](e) = G[w](v_j o_G)$ if $e \equiv o_{G_j} o_{G'}$ for some $j \in [m]$ and $T_j[w](e)$, where $e \in T_j[E]$, otherwise.
   (d) $G'[\sigma](v) = G[\sigma](o_G)$ if $v \equiv o_G$ and $T_j[\sigma](v)$, where $v \in T_j[V]$, otherwise.



(a) G (b) $G_1 \equiv T_{G_1}$ (c) $G_2 = T_{G_2}$

Figure 3: Construction of G'. G_1 and G_2 are the modified copies of G in step 2. In step 3, the transformation T_{G_i} happens to coincide with G_i for $i = 1, 2$ in this case. G' is created in step 4 by adding an extra vertex $o_{G'}$ and connecting it to v_1 and v_2 with the appropriate weights and activation and can be seen in Figure 1b.

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G' is well-defined We verify each steps in the above construction:

1. This step is well-defined.
2. For any G_j, as long as $\alpha_G \geq 2$ (by definition), we always remove o_G from each G_j in each step; since v_j is an in-vertex of o_G and G is a DAG. Otherwise, this step is well-defined.
3. Fix a $j \in [m]$. By construction (and since we always remove o_G from G_j in the previous step), $O_{G_j} = \{v_j\}$. If there is a path p^* with length at least t in G_j, then since $G_j[E] \subseteq G[E]$ and $o_G \in G[V] \setminus G_j[V]$, the path $p^* \cup \{o_G\}$ created by appending o_G to p^* is a valid path with length $t + 1$. This violates the assumption that $\alpha_G = t$ and we conclude, by contradiction, that $\alpha_{G_j} \leq t - 1$. This justifies the invocation of inductive hypothesis for ν_j to get a tree neural net τ_j.
4. The final step is well-defined.

ν' computes the same function as ν Recall that ν' is the neural network with graph G'. We have for any input $x \in \mathbb{R}^d$

$$\nu'(x) = (G'[\text{POST}](o_{G'}))(x) \tag{18}$$

$$= G'[\sigma](o_{G'}) \left(\sum_{j=1}^{m} G'[w](v_j o_{G'}) \cdot (G'[\text{POST}](v_j))(x) \right) \tag{19}$$

$$= G[\sigma](o_G) \left(\sum_{j=1}^{m} G[w](v_j o_G) \cdot (T_j[\text{POST}](v_j))(x) \right) \tag{20}$$

$$= G[\sigma](o_G) \left(\sum_{j=1}^{m} G[w](v_j o_G) \cdot (G[\text{POST}](v_j))(x) \right) = \nu(x) \tag{21}$$

where we invoked the inductive hypothesis in the last line to get

$$(T_j[\text{POST}](v_j))(x) = \tau_j(x) = \nu_j(x) = (G[\text{POST}](v_j))(x), \tag{22}$$

and the rest are definitions.

G' is isomorphic to T_G Although this should be straightforward from the construction, we give a formal proof. Consider the isomorphism $\pi : G'[V] \to T_G[V]$ given as

$$\pi(v) = \begin{cases} o_{T_G} = \{o_G\} \in \mathcal{H}_G & \text{if } v \equiv o_{G'} \\ p \cup \{o_G\} & \text{if } T_j[V] \ni v \equiv p \in \mathcal{H}_{G_j} \text{ for some } j \in [m], \end{cases} \tag{23}$$

where paths are viewed as set of vertices. The second case is well-defined since $p \cup \{o_G\} \in \mathcal{H}_G$ for any $p \in \mathcal{H}_{G_j}$ for any $j \in [m]$ by construction of G_j.

We can now verify that π is an isomorphism between the two structures. Fix $pq \in G'[E]$. Consider two separate cases: $pq \in T_j[E]$ for some j and $pq \notin T_j[E]$ for any j. In the first case, by definition of T_j as a Hasse diagram, $p = \{v_p\} \cup q$ are paths in $\mathcal{H}_{G_j}$. Thus, $\pi(p)\pi(q) = (p \cup \{o_G\})(q \cup \{o_G\})$ satisfying $\pi(p) = \{v_p\} \cup \pi(q)$. Thus, by definition of Hasse diagram, $\pi(p)\pi(q) \in T_G[E]$. Furthermore, $G'[w](pq) = G[w](e_p) = T_G[w](\pi(p)\pi(q))$ In the second case, we have $pq = v_j o_G$ for some $j \in [m]$. Thus, $\pi(p)\pi(q) = (\{v_j, o_G\})(\{o_G\}) \in T_G[E]$ also by definition of Hasse diagram. At the same time, $G'[w](pq) = G[w](v_j o_G) = T_G[w](\pi(p)\pi(q))$ by definition.

Fix $v \in G'[V]$. If $v \equiv o_{G'}$ then $G'[\sigma](v) = G[\sigma](o_G)$. At the same time, $T_G[\sigma](\pi(v)) = G[\sigma](v_{\{o_G\}} = G[\sigma](o_G) = G'[\sigma](v)$. If $v \not\equiv o_{G'}$ then there is a $j \in [m]$ and a $p \in \mathcal{H}_{G_j}$ such that $v = p \in T_j[V]$. Then by definition,

$$G'[\sigma](v) = T_j[\sigma](v) = G[\sigma](v_p) = G[\sigma](v_p \cup \{o_{G'}\}) = T_G[\sigma](\pi(v)). \tag{24}$$

This completes the inductive proof that shows $\tau_G = \nu' = \nu$ for G with $\alpha_G = t$. By mathematical induction, the claim holds for all neural network ν. □

Lemma 7 (Pull-back of numerical weights)**.** *Fix an arbitrary feedforward neural network $\nu : \mathbb{R}^d \to \mathbb{R}$ with computation graph G. Let $v \in G[V] \setminus (I_G \cup O_G)$ be an inner vertex of G with k in-edges $e_1, \ldots, e_k \in G[E]$ and a single out-edge $f \in G[E]$. Then the network ν' with computation graph $G' = (G[V], G[E], G'[w])$ defined as*

$$G'[w] : e \mapsto \begin{cases} G[w](e)|G[w](f)| & \textit{if } e \equiv e_j \textit{ for some } j \in [k] \\ \text{sgn}(G[w](f)) & \textit{if } e \equiv f \\ G[w](e) & \textit{otherwise.} \end{cases} \tag{25}$$

computes the same function as ν. In other words, we can pull the numerical values of $G[w](f)$ through v, into its in-edges; leaving behind only its sign.

When fixing input x to G, one can extend this operation to $i_j \in I_G$ for $j \in [d]$. By setting $G'[w](f) = \text{sgn}(G[w](f))$ and update x_j to $x_j|G[w](f)|$.

Proof. Let the single out-vertex of v be b. If suffices to show that $G[\text{PRE}](b) = G'[\text{PRE}](b)$. Fix an input x to ν. Let the k in-edges of v be $a_1, \ldots, a_k$. Since we only change edges incident to v, $G[\text{POST}]_{a_j} = G'[\text{POST}]_{a_j}$ for all $j \in [k]$. We have:

$$G'[\text{PRE}](b) = \text{sgn}(G[w](vb)) \cdot (G[\sigma](v))(G'[\text{PRE}](v)) \tag{26}$$

$$= \text{sgn}(G[w](vb)) \cdot (G[\sigma](v)) \left(\sum_{j=1}^{k} |G[w](vb)| G[w](a_j v) \cdot G[\text{POST}](a_j) \right) \tag{27}$$

$$= \text{sgn}(G[w](vb)) |G[w](vb)| \cdot (G[\sigma](v)) \left(\sum_{j=1}^{k} G[w](a_j v) \cdot G[\text{POST}](a_j) \right) \tag{28}$$

$$= G[w](vb) \cdot (G[\sigma](v)) \left(\sum_{j=1}^{k} G[w](a_j v) \cdot G[\text{POST}](a_j) \right) = G[\text{PRE}](b), \tag{29}$$

where equation 28 is due to positive homogeneity of σ_v and the rest are just definitions. □

We can now give the proof of Lemma 5.

Proof of Lemma 5. Given an arbitrary feedforward neural network ν with computation graph $G = (G[V], G[E], G[w])$, we use Lemma 6 and get the unrolled tree network $T_G = (T_G[V], T_G[E], T_G[w])$ such that $\nu = \tau_G$.

Let $\pi = \pi_1, \pi_2, \ldots, \pi_\xi$ be an ordering of $T_G[V] \setminus O_{T_G}$ (so $\xi = |\mathcal{H}| - 1$) by a breadth first search on T_G starting from o_{T_G}. In other words, if $d_{\text{topo}}(u, o_{T_G}) > d_{\text{topo}}(v, o_{T_G})$ then u appears after v in π, where $d_{\text{topo}}(a, b)$ is the number of edges on the unique path from a to b for some $a, b \in T_G[V]$. Iteratively apply Lemma 7 to vertex $\pi_1, \ldots, \pi_\xi$ in T_G while maintaining the same function. After ξ such applications, we arrive at a network μ'_G with graph M_G such that $\mu'_G = \tau_G = \nu$. Recall that the pull-back operation of Lemma 7 only changes the tree weights. Furthermore, the π ordering is chosen so that subsequent weight pull-back does not affect edges closer to o_{T_G}. Therefore, at iteration j,

1. $M_G[w](\pi_k q) = \text{sgn}(G[w](e_{\pi_k}))$ for all $k \leq j$, for some $q \in M_G[V]$ such that $(\pi_k)q \in M_G[E]$.
2. if $\pi_j \notin I_{M_G}$ then $M_G[w](r(\pi_j)) = G[w](e_r) \prod_{f \in \pi_j} |G[w](f)|$, for some $r \in M_G[V]$ such that $r(\pi_j) \in M_G[E]$; otherwise, π_j is an input vertex corresponding to input x_{π_j}, then x_{π_j} is modified to $x_{\pi_j} \prod_{f \in \pi_j} |G[w](f)| = h'_G(x_{\pi_j})$ where h'_G is the absolute-valued path enumeration function.

This completes the proof. □

Now we present the extension to Lemma 2:

Proof of Lemma 2. Invoke Lemma 5 to get a tree network μ' such that $\nu = \mu' \circ h'$. Then one can subdivide each input edges (edges that are incident to some input neuron i_j) into two edges connected by a neuron with linear activation. One of the resulting egde takes the weight of the old input edge; and the other is used to remove the absolute value in the definition of the (basic) path enumeration function.

More formally, for all $p \in \mathcal{P}$, recall that i_p is a particular input neuron of μ' in the decomposition lemma (Lemma 2). Since μ' is a tree neural network, we there exists a distinct node u_p in μ' that is adjacent to i_p. Remove the edge $i_p u_p$, add a neuron u'_p, connect $i_p u'_p$ and $u'_p u_p$, where the weight of the former neuron is set to $\text{sgn}\left(\prod_{e \in p} w_e\right)$ and the latter to $w[\mu'](i_p u_p)$. It is straightforward to see that with μ constructed from above, $\nu = \mu \circ h$ where h is the path enumeration function. □

With slight modifications to the proof technique, one can show all the results for Theorem 1, Theorem 2 and Corollary 1 to the same matrix representation as presented in the paper but with the absolute signs around them.

C PROOF OF TRAINING INVARIANCES

Claim 1 (Directional convergence to non-vanishing point implies stable sign)**.** *Assumption 2 implies Assumption 1.*

Proof. Let v be the direction that $\frac{w(t)}{\|w(t)\|_2}$ converges to. Let $\mathcal{O}$ be the orthant that v lies in. Since v does not have a 0 entry, the ball $\mathcal{B}$ with radius $\min_i |v_i|/2$ and center v is a subset of the interior of $\mathcal{O}$. Since $\frac{w(t)}{\|w(t)\|_2}$ converges to v, there exists a time T such that for all $s > T$, $\frac{w(s)}{\|w(s)\|_2} \in \mathcal{B}$. Thus, eventually, $w(s) \in \mathcal{B}$ where its signs stay constant. □

Claim 2 (Directional convergence does not imply stable activation)**.** *There exists a function $w : \mathbb{R} \to \mathbb{R}^d$ such that $w(t)$ converges in direction to some vector v but for all $u \in w(\mathbb{R})$, $w^{-1}(u)$ has infinitely many elements. This means that for some ReLU network empirical risk function $\mathcal{R}(w)$ whose set of nondifferentiable points D has nonempty intersection with $w(\mathbb{R})$, the trajectory $\{w(t)\}_{t\geq 0}$ can cross a boundary from one activation pattern to another an infinite number of times.*

Proof. Fix a vector $v \in \mathbb{R}^d$. Consider the function $t \mapsto v|t\sin(t)|$. □

Proof of Lemma 3. Recall that our real weight vector $w(t)$ is an arc Ji & Telgarsky (2020) which, by definition, is absolutely continuous. It then follows from real analysis that its component $w_e(t)$ is also absolutely continuous for any $e \in E$. For absolutely continuous functions $w_e(t)$ for some $e \in E$, invoke the Fundamental Theorem of Calculus (FTC) (Chapter 6, (Heil, 2019)), to get:

$$\sum_{u\in \mathrm{IN}_v} w_{uv}^2(t) - \sum_{u\in \mathrm{IN}_v} w_{uv}^2(0) = 2\sum_{u\in \mathrm{IN}_v} \int_{[0,t]} w_{uv}(s)\frac{\mathrm{d}w_{uv}}{\mathrm{d}t}(s)\mathrm{d}s \tag{30}$$

We now proceed to compute $\frac{\mathrm{d}w}{\mathrm{d}t}(s)$. Since $w(t)$ is absolutely continuous and we are taking the integral via FTC, we only need to compute $\frac{\mathrm{d}w}{\mathrm{d}t}(s)$ for a.e. time s. By chain rule (see for example, the first line of the proof of Lemma C.8 in Lyu & Li (2020)), there exists functions $(g_j)_{j=1}^n$ such that $g_j \in \partial\nu_{x_j}(w) \subseteq \mathbb{R}^{|E|}$ for all $j \in [n]$ where $\nu_{x_j}(w) = \nu(x_j; w)$, and for a.e. time $s \geq 0$,

$$\frac{\mathrm{d}w}{\mathrm{d}t}(s) = \frac{1}{n}\sum_{j=1}^{n} l'(y_j\nu(x_j; w(s)))\cdot y_j \cdot g_j \tag{31}$$

Fix $j \in [n]$, by the inclusion chain rule, since $\nu_{x_j} = \mu \circ h_{x_j}$, with h and μ also locally Lipschitz, we have by Theorem I.1 of Lyu & Li (2020),

$$\partial\nu_{x_j}(w) = \partial(\mu\circ h_{x_j})(w) \subseteq \mathrm{CONV}\left\{\sum_{p\in\rho}[\alpha]_\rho\beta_{j,\rho} \mid \alpha \in \partial\mu(h(w)), \beta_{j,\rho} \in \partial[h_{x_j}]_p(w)\right\}. \tag{32}$$

Thus there exists $(\gamma_a)_{a=1}^A \geq 0, \sum_{a=1}^A \gamma_a = 1$ and $(\alpha^a \in \partial\mu(h(w)), \beta_{j,p}^a \in \partial[h_{x_j}]_p(w))_{a=1}^A$ such that:

$$g_j = \sum_{a=1}^{A}\gamma_a\sum_{p\in\rho}[\alpha^a]_p\beta_{j,p}^a.$$

Here we use Assumption 1 to deduce that eventually, all weights are non-zero in gradient flow trajectory to compute:

$$\partial[h_{x_j}]_p(w) = \left\{\frac{\mathrm{d}[h_{x_j}]_p(w)}{\mathrm{d}(w)}\right\} = \left\{\left(\mathbb{1}_{e\in p}\cdot \mathrm{sgn}(w_e)\cdot(x_j)_p\prod_{f\in p, f\neq e}|w_f|\right)_{e\in E}\right\}.$$

Plug this back into g_j to get:

$$g_j = \left(\sum_{a=1}^{A} \gamma_a \sum_{p \in \rho | e \in p} [\alpha]_p^a \text{sgn}(w_e) \cdot (x_j)_p \prod_{f \in p, f \neq e} |w_f| \right)_{e \in E}.$$

Plug this back into $\frac{\mathrm{d}w}{\mathrm{d}t}(s)$ and to get, coordinate-wise, for a.e. $s \geq 0$,

$$\frac{\mathrm{d}w_e}{\mathrm{d}t}(s) = \frac{1}{n} \sum_{j=1}^{n} l'(y_i \nu(x_i; w(s))) \cdot y_i \cdot \sum_{a=1}^{A} \gamma_a \sum_{p \in \rho | e \in p} [\alpha^a]_p \text{sgn}(w_e(s)) \cdot (x_j)_p \prod_{f \in p, f \neq e} |w_f(s)|. \quad (33)$$

Multiply both sides with w_e gives:

$$w_e(s) \frac{\mathrm{d}w_e}{\mathrm{d}t}(s) = \sum_{p \in \mathcal{P} | e \in p} \frac{1}{n} \sum_{j=1}^{n} d_{j,p}(w(s)), \quad (34)$$

where

$$d_{j,p}(w) = l'(y_i \nu(x_i; w)) \cdot y_i \cdot \sum_{a=1}^{A} \gamma_a [\alpha]_p^a \cdot (x_j)_p \cdot \prod_{f \in p} |w_f(s)|. \quad (35)$$

Note that d does not depend on the specific edge e used in Equation 33.

Plugging back into the FTC to get:

$$\sum_{u \in \text{IN}_v} w_{uv}^2(t) - \sum_{u \in \text{IN}_v} w_{uv}^2(0) = 2 \sum_{u \in \text{IN}_v} \int_{[0,t]} \sum_{p \in \mathcal{P} | uv \in p} \frac{1}{n} \sum_{j=1}^{n} d_{j,p}(w(s)) \mathrm{d}s \quad (36)$$

$$= 2 \int_{[0,t]} \sum_{p \in \mathcal{P} | v \in p} \frac{1}{n} \sum_{j=1}^{n} d_{j,p}(w(s)) \mathrm{d}s. \quad (37)$$

Finally, by an identical argument but applied to the set of edges $vb$for some $b \in \text{OUT}_v$, we have:

$$\sum_{b \in \text{OUT}_v} w_{vb}^2(t) - \sum_{b \in \text{OUT}_v} w_{vb}^2(0) = 2 \int_{[0,t]} \sum_{p \in \mathcal{P} | v \in p} \frac{1}{n} \sum_{j=1}^{n} d_{j,p}(w(s)) \mathrm{d}s \quad (38)$$

$$= \sum_{u \in \text{IN}_v} w_{uv}^2(t) - \sum_{u \in \text{IN}_v} w_{uv}^2(0), \quad (39)$$

which completes the proof of the first part of the lemma.

For the second part, recall that we have 2 vertices u, v such that $\text{IN}_v = \text{IN}_u = \text{IN}$ and $\text{OUT}_v = \text{OUT}_u = \text{OUT}$. Use 33 to get, for notations set up previously, for almost every time $s > 0$,

$$\sum_{a \in \text{IN}} \text{sgn}(w_{au}(s) w_{av}(s)) \left(w_{au}(s) \frac{\mathrm{d}w_{av}}{\mathrm{d}t}(s) + \frac{\mathrm{d}w_{au}}{\mathrm{d}t}(t) w_{av}(t) \right) = \sum_{p \in \mathcal{A}} \frac{1}{n} \sum_{j=1}^{n} d_{j,p}(w(s)), \quad (40)$$

where $\mathcal{A}$ is a set of jagged paths (Figure 4) defined as

$$\mathcal{A} = \left\{ p_1 \cup p_2 | p_1 \text{ is a path from } I \text{ to } v \text{ or } u; p_2 \text{ is a of path from } u \text{ or } v, \text{ respectively, to } O \right\}.$$

Then by a double counting argument, we also have

$$\sum_{b \in \text{OUT}} \text{sgn}(w_{ub}(s) w_{vb}(s)) \left(w_{ub}(t) \frac{\mathrm{d}w_{vb}}{\mathrm{d}t}(t) + \frac{\mathrm{d}w_{ub}}{\mathrm{d}t}(t) w_{vb}(t) \right) \quad (41)$$

$$= \sum_{p \in \mathcal{A}} \frac{1}{n} \sum_{j=1}^{n} d_{j,p}(w(s)) \quad (42)$$

$$= \sum_{a \in \text{IN}} \text{sgn}(w_{au}(s) w_{av}(s)) \left(w_{au}(t) \frac{\mathrm{d}w_{av}}{\mathrm{d}t}(t) + \frac{\mathrm{d}w_{au}}{\mathrm{d}t}(t) w_{av}(t) \right). \quad (43)$$

Integrate both sides over $[0, t]$ as we did in the first part to get the conclusion of the second part. Note that the second part is special case of the first part, which is obtainable by setting $u = v$. We point out that proof of the first and second part of this lemma differs only in the choice of the set $\mathcal{A}$ (in the first part, $\mathcal{A}$ is the set of all paths that goes through v). □

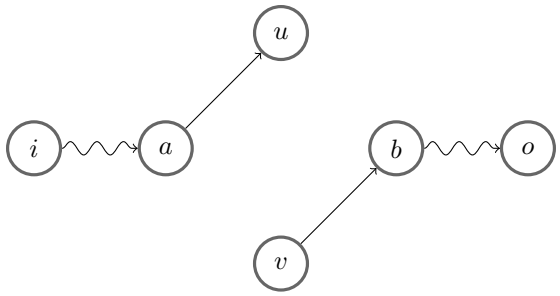

Figure 4: Jagged path. Here the straight arrow denote a single edge in the graph while the snaked arrow denote a path with possibly more than one edge. u and v are nodes in the statement of the second part of Lemma 3, $a \in \text{IN} = \text{IN}_v = \text{IN}_u$, $b \in \text{OUT} = \text{OUT}_v = \text{OUT}_u$.

Proof of Lemma 4. The proof is identical to that of Lemma 3, with the only difference being the set $\mathcal{A}$ that we double count. Here, set $\mathcal{A}$ to be $\mathcal{P}$. Then by the definition of layer (see Definition 6), one can double count $\mathcal{P}$ by counting paths that goes through any element of a particular layer. The proof completes by considering (using the same notation as the proof of Lemma 3) for a.e. time $s \geq 0$,

$$\sum_{e \in F} w_e(s) \frac{\mathrm{d}w_e}{\mathrm{d}t}(s) = \sum_{p \in \mathcal{P}} \frac{1}{n} \sum_{j=1}^{n} d_{j,p}(w(s)) \cdot (x_j)_p \cdot \prod_{f \in p} |w_f(s)|, \tag{44}$$

for any layer F. □

Before continuing with the proof of Theorem 1, we state a classification of neurons in a convolutional layer. Due to massive weight sharing within a convolutional layer, there are a lot more neurons and edges than the number of free parameters in this layer. Here, we formalize some concepts:

Definition 10 (Convolutional tensors)**.** *Free parameters in a (bias-free) convolutional layer can be organized into a tensor $T \in R^{a \times b \times c}$ where a is the number of input channels, b is the size of each 2D filter and c is the number of output channels.*

For example, in the first convolutional layer of AlexNet, the input is an image with 3 image channels (red, blue and green), so $a = 3$ in this layer; filters are of size 11×11 so $b = 121$ is the size of each 2D filter; and finally, there are 96 output channels, so $c = 96$. Note that changing the stride and padding does not affect the number of free parameters, but does change the number of neurons in the computation graph of this layer. Thus, we need the following definition:

Definition 11 (Convolutional neuron organization)**.** *Fix a convolutional layer with free parameters $T \in R^{c \times b \times a}$. Then neurons in this layer can be organized into a two dimensional array $\{v_{j,k}\}_{j \in [l], k \in [c]}$ for some $l \in \mathbb{N}$ such that*

1. *For all $j, j' \in [l]$ and for all $k \in [c]$, $v_{j,k}$ and $v_{j',k}$ share all its input weights. More formally, there exists a bijection $\phi : \text{IN}_{v_{j,k}} \to \text{IN}_{v_{j',k}}$ such that:*

$$w_{uv_{j,k}} \equiv w_{\phi(u)v_{j',k}}, \tag{45}$$

   for all $u \in \text{IN}_{v_{j_k}}$.

2. *For all $j \in [l]$ and for all $k, k' \in [c]$, $v_{j,k}$ and $v_{j,k'}$ has the same in-vertices and out-vertices. In other words,*

$$\text{IN}_{v_{j_k}} = \text{IN}_{v_{j,k'}} =: \text{IN}_{v_j} \text{ and } \text{OUT}_{v_{j_k}} = \text{OUT}_{v_{j,k'}} =: \text{OUT}_{v_j}. \tag{46}$$

For example, in the first convolutional of AlexNet in $\mathbb{R}^{96\times 121\times 3}$, the input image dimension is $224 \times 224 \times 3$ pixels and the stride of the $11 \times 11 \times 3$ filters in the layer is 4, with no padding. Thus a single 2D filter traverse the image $\left(\frac{224-(11-4)}{4}\right)^2 =: l$ times, each corresponds to a different neuron in the layer. This process is then repeated c times for each output channel, for a total of $c \times l$ neurons in the convolutional layer.

Lemma 8 (Extension of Lemma 3 to weight sharing)**.** *Let $\mathcal{V} := \{v_{j,k}\}_{j\in[l],k\in\{1,2\}}$ be a convolutional neuron organization. Recall that by definition 11, for all $j \in [l]$, $\text{IN}_{v_{j,1}} = \text{IN}_{v_{j,2}} =: \text{IN}_j$ and $\text{OUT}_{v_{j,1}} = \text{OUT}_{v_{j,2}} =: \text{OUT}_j$. We have for a.e. time $t \geq 0$,*

$$\sum_{(w,w')\in w_{\text{IN}}(\mathcal{V})} |w(t)w'(t)| - |w(0)w'(0)| = \sum_{(z,z')\in w_{\text{OUT}}(\mathcal{V})} |z(t)z'(t)| - |z(0)z'(0)|, \tag{47}$$

where

$$w_{\text{IN}}(\mathcal{V}) := \{(w_1, w_2) \mid \forall j \in [l], \exists a_j \in \text{IN}_j, w_{a_j v_{j,1}} \equiv w_1 \text{ and } w_{a_j v_{j,2}} \equiv w_2\},$$

and similarly,

$$w_{\text{OUT}}(\mathcal{V}) := \{(w_1, w_2) \mid \forall j \in [l], \exists b_j \in \text{OUT}_j, w_{v_{j,1} b_j} \equiv w_1 \text{ and } w_{v_{j,2} b_j} \equiv w_2\}.$$

Before we start the proof, some remarks are in order. Let $T_1 \in \mathbb{R}^{2\times b\times a}$ be a convolutional layer and let $\mathcal{V} = \{v_{j,k}\}_{j\in[l],k\in[2]}$ be its convolutional neuron organization. Then

$$w_{\text{IN}}(\mathcal{V}) = \{([T_1]_{1,j_2,j_1}, [T_1]_{2,j_2,j_1}) \mid j_1 \in [a], j_2 \in [b]\}. \tag{48}$$

If furthermore $T_2 \in R^{e\times d\times 2}$ is a convolutional layer immediately after T_1, then

$$w_{\text{OUT}}(\mathcal{V}) = \{([T_2]_{k_1,k_2,1}, [T_2]_{k_1,k_2,2}) \mid k_1 \in [e], k_2 \in [d]\}. \tag{49}$$

If instead of T_2, the subsequent layer to T_1 is a fully-connected layer $W \in \mathbb{R}^{d\times(l\times 2)}$ (recall that there are $2l$ neurons in T_1 layer), then

$$w_{\text{OUT}}(\mathcal{V}) = \{(W_{l_1,l_2\times 1}, [T_2]_{l_1,l_2\times 2}) \mid l_1 \in [d], l_2 \in [l]\}. \tag{50}$$

Proof of Lemma 8. As before, the proof is identical to that of Lemma 3 with the exception being the set of paths that we are double counting over. For all $j \in [l]$, let

$$\mathcal{A}_j := \{p_1 \cup p_2 \mid p_1 \text{ is a path from } I \text{ to } v_{j,1}\ , p_2 \text{ is a path from } v_{j,2} \text{ to } o\}, \tag{51}$$

and

$$\mathcal{A}'_j := \{p_1 \cup p_2 \mid p_1 \text{ is a path from } I \text{ to } v_{j,2}\ , p_2 \text{ is a path from } v_{j,1} \text{ to } o\}. \tag{52}$$

Let $\mathcal{A} := \bigcup_{j\in[l]} \mathcal{A}_j \cup \mathcal{A}'_j$. Then by an identical argument as that of Lemma 3, we can show that

$$\sum_{(w,w')\in w_{\text{IN}}(\mathcal{V})} |w(t)w'(t)| - |w(0)w'(0)| = \int_{[0,t]} \sum_{p\in\mathcal{A}} \frac{1}{n} \sum_{j=1}^{n} d_{j,p}(w(s))\mathrm{d}s \tag{53}$$

$$= \sum_{(z,z')\in w_{\text{OUT}}(\mathcal{V})} |z(t)z'(t)| - |z(0)z'(0)|. \tag{54}$$

□

Proof of Theorem 1. All points in this theorem admit the same proof technique: First, form the matrices as instructed. Let $X = \{v_1, v_2, \ldots, v_m\} \subseteq V$ be the neurons shared between the two layers. Check the conditions of the second part of Lemma 3 and invoke the lemma for each pair $u, v \in X$. We now apply this to each points:

1. Let $W_1 \in \mathbb{R}^{b\times a}$ be a fully-connected layer from neurons in V_1 to neurons in V_2 and $W_2 \in \mathbb{R}^{c\times b}$ be a fully-connected layer from V_2 to V_3. Then we have $\text{IN}_u = V$ and $\text{OUT}_u = W$ for all $u \in U$. Furthermore, all weights around any u are learnable for all u in U. Invoke the second part of Lemma 3 to get the conclusion.

2. let $T_1 \in \mathbb{R}^{c\times b\times a}$ and $T_2 \in \mathbb{R}^{e\times d\times c}$ be the convolutional tensors with convolutional neuron organization of T_1 (Definition 11) being $\{v_{j,k}\}_{j\in[l_1],k\in[c]}$. Form the matrix representation $W_1 \in \mathbb{R}^{c\times(ab)}$ and $W_2 \in \mathbb{R}^{(de)\times c}$ as per the theorem statement. By Definition 11, for $k, k' \in [c]$, for all $j \in [l]$, $\text{IN}_{v_{j,k}} = \text{IN}_{v_{j,k'}}$ and $\text{OUT}_{v_{j,k}} = \text{OUT}_{v_{j,k'}}$. Invoke Lemma 8 to get the conclusion.

3. Let $r(x; U, Y, Z)$ be a residual block of either ResNetIdentity, ResNetDiagonal or ResNetFree. In all variants, skip connection affects neither the edges in $U \in \mathbb{R}^{b\times a}$ and $Y \in \mathbb{R}^{c\times b}$. Let Y be fully-connected from neurons V_1 to neurons V_2 and U be fully-connected from neurons V_2 to neurons V_3. Then for each $u \in V_2$, $\text{IN}_u = V_1$ and $\text{OUT}_u = V_3$. Furthermore, all weights around any vertices in V_2 are learnable. Invoke the second part of Lemma 3 to get the conclusion.

4. Let $r_i(x; U_i, Y_i, Z_i), i \in \{1, 2\}$ be consecutive ResNetFree block. Let Y_1 be fully connected from neurons V_1 to neurons V_2, U_1 be fully-connected from V_2 to neurons V_3, Y_2 be fully-connected from neurons V_3 to V_4 and U_2 be fully-connected from V_4 to neurons V_5. Then $\begin{bmatrix} U_1 & Z_1 \end{bmatrix}$ is fully-connected from $V_1 \cup V_2$ to V_3 and $\begin{bmatrix} Y_2 \\ Z_2 \end{bmatrix}$ is fully-connected from V_3 to $V_4 \cup V_5$. Invoke the first point to get the conclusion.

5. Let the convolutional tensor be $T \in \mathbb{R}^{c\times b\times a}$ with convolutional neuron organization $\{v_{j,k}\}_{j\in[l],k\in[c]}$ for some $l \in \mathbb{N}$. Let the adjacent fully-connected layer be $W \in \mathbb{R}^{d\times(l\times c)}$. Form the matrix representation $W_1 \in \mathbb{R}^{c\times ab}$ and $W_2 \in \mathbb{R}^{dl\times c}$ as per the theorem statement. Then we have for any $k, k' \in [c]$ and for all $j \in [l]$, $\text{IN}_{v_{j,k}} = \text{IN}_{v_{j,k'}} =: \text{IN}_j$ and $\text{OUT}_{v_{j,k}} = \text{OUT}_{v_{j,k'}} =: \text{OUT}_j$. Invoke Lemma 8 to get the conclusion.

6. Let $r(x; U, Y, Z)$ be a residual block of either ResNetIdentity, ResNetDiagonal or ResNetFree. Let Y be fully-connected from neurons V_1 to neurons V_2, U be fully-connected from neurons V_2 to neurons V_3. Thus, Z is fully-connected from V_1 to V_3. Then $W_2 = \begin{bmatrix} U & Z \end{bmatrix}$ is fully connected from V_1 to $V_2 \cup V_3$.We invoke the fifth point to get the conclusion.

7. first consider the case where the ResNetFree block is followed by the fully-connected layer. Let $r(x; U, Y, Z)$ be the first ResNetFree block with input neurons where Y fully-connects neurons V_1 to V_2 and U fully connects V_2 to V_3. Then we have $\begin{bmatrix} U & Z \end{bmatrix}$ fully-connects $V_1 \cup V_2$ to V_3. If the subsequent layer is a fully-connected layer then invoke the first point to get the conclusion; otherwise if the subsequent layer is a ResNetFree block $r(x; U', Y', Z')$ with Y' fully-connects V_3 to V_4 and U' fully-connects V_4 to V_5. Then $\begin{bmatrix} Y \\ Z \end{bmatrix}$ fully-connects V_3 to $V_4 \cup V_5$ and we one again invoke the first point to get the conclusion.

□

D PROOF OF THEOREM 2

First we state a helper lemma

Lemma 9 (Largest singular value of different flattening of the same tensor is close)**.** *Let $T \in \mathbb{R}^{a,b,c}$ be an order 3 tensor (say a convolutional weight tensor). Let T_1, T_2 be the standard flattening of this tensor into an element in $\mathbb{R}^{c\times(a\times b)}$ and $\mathbb{R}^{(b\times c)\times a}$ respectively. Then,*

$$\frac{1}{\min(a, b)}\|T_1\|_2^2 \leq \|T_2\|_2^2. \tag{55}$$

Proof. Invoke Theorem 4.8 of Wang et al. (2017) and using the same notation in the same paper, we have for $\pi_1 = \{\{c\}, \{a, b\}\}$ and $\pi_2 = \{\{b, c\}, \{a\}\}$,

$$\frac{\dim_T(\pi_1, \pi_2)}{\dim(T)}\|T_1\|_2^2 \leq \|T_2\|_2^2. \tag{56}$$

All that is left is to compute the left hand side in term of a, b, c. By definition, $\dim(T) = abc$ and

$$\dim_T(\pi_1, \pi_2) = \dim_T(\{\{c\}, \{a, b\}\}, \{\{b, c\}, \{a\}\}) \tag{57}$$
$$= \Big[\max\big(D_T(\{c\}, \{b, c\}), D_T(\{c\}, \{a\})\big)\Big] \tag{58}$$
$$\cdot \Big[\max\big(D_T(\{a, b\}, \{b, c\}), D_T(\{a, b\}, \{a\})\big)\Big] \tag{59}$$
$$= \big[\max(c, 0)\big] \cdot \big[\max(a, b)\big] = c\max(a, b). \tag{60}$$

Plug this in equation 56 to get the final result. □

Lemma 10 (Shuffling layer in ResNetFree block preserves largest singular value up to multiple by 8)**.** *Recall that for a ResNetFree block $r(U, Y, Z)$ with $Y \in \mathbb{R}^{b\times a}$, $U \in \mathbb{R}^{c\times b}$ and $Z \in \mathbb{R}^{c\times a}$, there are two possible rearrangement of the weights $A = \begin{bmatrix} U & Z \end{bmatrix}$ and $B = \begin{bmatrix} Y \\ Z \end{bmatrix}$. We have $\|B\|_2^2 \geq \frac{1}{8}\|A\|_2^2 - D'$ where $D' \geq 0$ is fixed at inialization.*

Proof. Recall that by point three of Theorem 1, we have matrix invariance

$$U^\top(t)U(t) - Y(t)Y^\top(t) = U^\top(0)U(0) - Y(0)Y^\top(0).$$

By line $B.2$ in Ji & Telgarsky (2019),

$$\|Y\|_2^2 \geq \|U\|_2^2 - D, \tag{61}$$

where $D = \|U^\top(0)U(0) - Y(0)Y^\top(0)\|_2^2$ is fixed at initialization.

For positive semidefinite matrix X, denote $\lambda(X)$ to be the function that returns the maximum eigenvalue of X. We have

$$\|B\|_2^2 = (\lambda(B^\top B))^2 \tag{62}$$
$$= \left(\lambda\left(Y^\top Y + Z^\top Z\right)\right)^2 \tag{63}$$
$$\geq \frac{1}{4}\left(\lambda\left(Y^\top Y\right) + \lambda\left(Z^\top Z\right)\right)^2 \tag{64}$$
$$\geq \frac{1}{4}\left(\lambda\left(Y^\top Y\right)\right)^2 + \frac{1}{4}\left(\lambda\left(Z^\top Z\right)\right)^2 \tag{65}$$
$$\geq \frac{1}{4}\left(\lambda\left(UU^\top\right)\right)^2 + \frac{1}{4}\left(\lambda\left(ZZ^\top\right)\right)^2 - \frac{D}{4} \tag{66}$$
$$\geq \frac{1}{8}\left(\lambda\left(UU^\top\right) + \lambda\left(ZZ^\top\right)\right)^2 - \frac{D}{4} \tag{67}$$
$$\geq \frac{1}{8}\left(\lambda\left(UU^\top + ZZ^\top\right)\right)^2 - \frac{D}{4} \tag{68}$$
$$= \frac{1}{8}\left(\lambda\left(AA^\top\right)\right)^2 - \frac{D}{4} = \frac{1}{8}\|A\|_2^2 - \frac{D}{2}, \tag{69}$$

where 64 is by an application of Weyl's inequality for Hermitian matrices which states that $\lambda(C + D) \geq \lambda(C) + t$ where t is is the smallest eigenvalue of D, which is nonnegative since matrices here are all positive semidefinite; 66 is a consequence of 61 and 68 is the application of the inequality $\lambda(C + D) \leq \lambda(C) + \lambda(D)$ which is another of Weyl's inequality for Hermitian matrices. □

Proof of Theorem 2. Fix $j \in [K + M]$, similar to the proof of Theorem 1, we first invoke Lemma 4 to bound the Frobenius norm of each of the final $K + M + 1$ layers (counting the last layer Fin) via the last layer. Let W_j be the matrix representation of the j-th layer among the last $M + 1$ layer as described in Theorem 1. Note that even if a layer has more than one matrix representation

in Theorem 1, their Frobenius norm is still the same because different representation merely reorganize the weights. Thus, we can pick an arbitrary representation in this step. However, the same is not true for the operator norm and we have to be a lot more careful in the next step. For each $j \in [K+M]$, we have

$$\|W_j(t)\|_F^2 - \|Fin(t)\|_F^2 = D_0, \tag{70}$$

where $D_0 = \|W_j(0)\|_F^2 - \|Fin(0)\|_F^2$ fixed at initialization.

Now, similar to the proof of Theorem 1, we bound the difference between the operator norm of $W_j(t)$ and $Fin(t)$ by a telescoping argument. By Lemma 10, switching from one matrix representation to the other for ResNet incurs at most a multiplicative factor of 8 and an additive factor cost that depends only on the initialization. In each adjacent layer, the maximum number of switch between representation is one (so that it fits the form prescribed in Theorem 1). By matrix invariance between adjacent layers of the $K+M$ pairs of adjacent layers,

$$\|W_l(t)\|_2^2 \geq C\|W_{l+1}(t)\|_2^2 - D_l, \tag{71}$$

for $C = 1/8$ if the $k+1$ layer is a ResNetFree block (Lemma 10), $C = 1/\min(a_{k+1}, b_{k+1})$ if the $k+1$ layer is a convolutional layer, $C = \max \dim W^{[M+1]}$ if $k = M$ (Lemma 9) and $C = 1$ otherwise; for $D_l = \|W_{l+1}^\top(0)W_{l+1}(0) - W_l(0)W_l^\top(0)\|_2^2$.

Telescope the sum and subtract from 70 to get the statement of the theorem. When Frobenius norm diverges, divide both sides by the Frobenius norm to get the ratio statement. Note that the bound $\|W\|_F^2/\text{rank}(W) \leq \|W\|_2^2$ is trivial since the largest singular value squared is at least the average singular value squared.

When the lower bound of 14 is 1, it matches the upper bound and thus the largest singular value dominates all other singular values. Alignment follows from the proof of Lemma 2.6 second point in Ji & Telgarsky (2019). □

E Proof of Corollary 1

Proof. Let L be the number of layers in the network. Under the conditions stated in Corollary 1, Lyu & Li (2020) and Ji & Telgarsky (2020) showed that $\|w(t)\|_2$ diverges. Invoke Lemma 4 for all $k \in [L-1]$ and sum up the results, we have $L\|W_L(t)\|_F^2 = D'' + \sum_{j=1}^L \|W_j(t)\|_F^2 \; \|W_k\|_F^2 = D'' + \|w(t)\|_2^2$ where D'' is constant in t. Thus $\|W_j(t)\|_F^2$ diverges for all $j \in [L]$. Since the sum of all but the largest singular value is bounded, but the sum of all singular values diverge, we conclude that the largest singular value eventually dominates the remaining singular values. Together with convergence in direction for these architecture Ji & Telgarsky (2020), we have each matrix converges to its rank-1 approximation.

That all the feedforward neural networks with ReLU/leaky ReLU/linear activations can be definable in the same o-minimal structure that contains the exponential function follows from the work of Ji & Telgarsky (2020) and that definability is closed under function composition. □

F Extension to gradient descent

Recall that with gradient descent for some step size $\eta : \mathbb{N} \to \mathbb{R}_{\geq 0}$, the weight trajectory is a solution to the system of finite differences:

$$w(t+1) - w(t) = -\eta(t)d(w(t)), \tag{72}$$

for some $\{d(w(t)) \in \partial\mathcal{R}(w(t))\}_{t\in\mathbb{N}}$ sequence of subgradient choice at each time step. This section essentially recovers Ji & Telgarsky (2019) extension of deep linear network results to gradient descent.

From 72, for some $\{d(w(t)) \in \partial\mathcal{R}(w(t))\}_{t\in\mathbb{N}}$, we have,

$$w(t+1)w(t) - w(t)^2 = -\eta(t)w(t)d(w(t)) \tag{73}$$

$$w(t+1)^2 + w(t)^2 - 2w(t+1)w(t) = \eta(t)^2 d(w(t))^2, \tag{74}$$

by multiplying both sides with $w(t)$ or squaring both sides respectively.

Combine the above two equations to get:

$$w(t+1)^2 - w(t)^2 - \eta(t)^2 d(w(t))^2 = -2\eta(t)w(t)d(w(t)). \tag{75}$$

Take a telescoping sum to get:

$$w(t+1)^2 - w(0)^2 - \sum_{\tau=0}^{t} \eta(\tau)^2 d(w(\tau))^2 = -2\sum_{\tau=0}^{t} \eta(\tau)w(\tau)d(w(\tau)). \tag{76}$$

Fix an edge e and recall that we had from the proof of Theorem 1 that, for all $s \in \mathbb{N}$,

$$w_e(s)[d(w(s))]_e = \sum_{p\in\mathcal{P}|e\in p} \frac{1}{n}\sum_{j=1}^{n} d_{j,p}(w(s)). \tag{77}$$

Therefore, fix a vertex v satisfying the conditions in Theorem 1, we have,

$$\sum_{u\in \text{IN}_v} w_{uv}(t+1)^2 - w_{uv}(0)^2 - \sum_{\tau=0}^{t} \eta(\tau)^2 [d(w(\tau))]_{uv}^2 \tag{78}$$

$$= -2\sum_{\tau=0}^{t} \eta(\tau) \sum_{p\in\mathcal{P}|v\in p} \frac{1}{n}\sum_{j=1}^{n} d_{j,p}(w(\tau)) \tag{79}$$

$$= \sum_{b\in \text{IN}_v} w_{vb}(t+1)^2 - w_{vb}(0)^2 - \sum_{\tau=0}^{t} \eta(\tau)^2 [d(w(\tau))]_{vb}^2. \tag{80}$$

which recovers a vertex-wise invariance with some slack terms. With an identical argument, we can recover the second part of Theorem 1 as well:

$$\sum_{a\in \text{IN}} w_{av}(t+1)w_{au}(t+1) - w_{av}(0)w_{au}(0) - \sum_{\tau=0}^{t} \eta(\tau)^2 [d(w(\tau))]_{av}[d(w(\tau))]_{au} \tag{81}$$

$$= -2\sum_{\tau=0}^{t} \eta(\tau) \sum_{a\in \text{IN}} w_{av}(\tau)[d(w(\tau))]_{au} + w_{au}(\tau)[d(w(\tau))]_{av} \tag{82}$$

$$= -2\sum_{\tau=0}^{t} \eta(\tau) \sum_{p\in\mathcal{A}} \frac{1}{n}\sum_{j=1}^{n} d_{j,p}(w(\tau)) \tag{83}$$

$$= -2\sum_{\tau=0}^{t} \eta(\tau) \sum_{b\in \text{OUT}} w_{vb}(\tau)[d(w(\tau))]_{ub} + w_{ub}(\tau)[d(w(\tau))]_{bv} \tag{84}$$

$$= \sum_{b\in \text{IN}_v} w_{vb}(t+1)w_{ub}(t+1) - w_{vb}(0)w_{ub}(0) - \sum_{\tau=0}^{t} \eta(\tau)^2 [d(w(\tau))]_{vb}[d(w(\tau))]_{ub}. \tag{85}$$

We thus recover the matrix invariance of Ji & Telgarsky (2019) equation C.9.

To control singular values of adjacent layers' matrix representations, we needs to control the growth of the slack term using the step size η. One way to do this is to adaptively set the step size based on the Frobenius norm of each layer. Let us assume that at time step t, the maximum Frobenius norm of any layer is $R(t)$ and that the risk $\mathcal{R}$ (as a function of time) has $\beta(t)$-Lipschitz gradient (or is $\beta(t)$-smooth) in this Frobenius norm ball. Then by smoothness of $\mathcal{R}$, setting $\eta(\tau) = \min\left(1, \frac{1}{\beta(\tau)}\right)$ for any $\tau \in \mathbb{N}$, we have,

$$\mathcal{R}(w(\tau)) - \mathcal{R}(w(\tau+1)) \leq \left\langle d(w(\tau)), -\eta(t)d(w(\tau))\right\rangle + \frac{\beta(\tau)\eta(\tau)^2}{2}\|d(w(\tau))\|_2^2 \tag{86}$$

$$= -\frac{\eta(\tau)}{2}\|d(w(\tau))\|_2^2. \tag{87}$$

Therefore,

$$\mathcal{R}(w(0)) \leq \mathcal{R}(w(0)) - \mathcal{R}(w(t+1)) \leq -\frac{1}{2}\sum_{\tau=0}^{t} \eta(\tau)\|d(w(\tau))\|_2^2 \tag{88}$$

$$\leq -\frac{1}{2}\sum_{\tau=0}^{t} \eta(\tau)^2\|d(w(\tau))\|_2^2 \tag{89}$$

$$\leq -\frac{1}{2}\sum_{\tau=0}^{t} \eta(\tau)^2[d(w(\tau))]_e[d(w(\tau))]_f. \tag{90}$$

for any $e, f \in E$. Therefore we conclude that the slack term is bounded by a quantity that is fixed at initialization. This allows us to recover Theorem 2 and Corollary 1 for gradient descent (but note that here we have an extra assumption in term of the smoothness of the risk function).