Luck Matters: Understanding Training Dynamics of Deep ReLU Networks

Abstract
We analyze the dynamics of training deep ReLU networks and their implications on generalization capability. Using a teacher-student setting, we discovered a novel relationship between the gradient received by hidden student nodes and the activations of teacher nodes for deep ReLU networks. With this relationship and the assumption of small overlapping teacher node activations, we prove that (1) student nodes whose weights are initialized to be close to teacher nodes converge to them at a faster rate, and (2) in over-parameterized regimes and 2-layer case, while a small set of lucky nodes do converge to the teacher nodes, the fan-out weights of other nodes converge to zero. This framework provides insight into multiple puzzling phenomena in deep learning like over-parameterization, implicit regularization, lottery tickets, etc. We verify our assumption by showing that the majority of BatchNorm biases of pre-trained VGG11/16 models are negative. Experiments on (1) random deep teacher networks with Gaussian inputs, (2) teacher network pre-trained on CIFAR-10 and (3) extensive ablation studies validate our multiple theoretical predictions.

1. Introduction
Although neural networks have made strong empirical progress in a diverse set of domains (e.g., computer vision (16; 32; 10), speech recognition (11; 1), natural language processing (22; 3), and games (30; 31; 35; 23)), a number of fundamental questions still remain unsolved. How can Stochastic Gradient Descent (SGD) find good solutions to a complicated non-convex optimization problem? Why do neural networks generalize? How can networks trained with SGD fit both random noise and structured data (38; 17; 24), but prioritize structured models, even in the presence of massive noise (27)? Why are flat minima related to good generalization? Why does over-parameterization lead to better generalization (25; 39; 33; 26; 19)? Why do lottery tickets exist (6; 7)?

In this paper, we propose a theoretical framework for multilayered ReLU networks. Based on this framework, we try to explain these puzzling empirical phenomena with a unified view. We adopt a teacher-student setting where the label provided to an over-parameterized deep student ReLU network is the output of a fixed teacher ReLU network of the same depth and unknown weights (Fig. 1(a)). In this perspective, hidden student nodes are randomly initialized with different activation regions. (Fig. 2(a)). During optimization, student nodes compete with each other to explain teacher nodes. Theorem 4 shows that lucky student nodes which have greater overlap with teacher nodes converge to those teacher nodes at a fast rate, resulting in winner-take-all behavior. Furthermore, Theorem 5 shows that if a subset of student nodes are close to the teacher nodes, they converge to them and the fan-out weights of other irrelevant nodes of the same layer vanishes.

With this framework, we can explain various neural network behaviors as follows:

Fitting both structured and random data. Under gradient descent dynamics, some student nodes, which happen to overlap substantially with teacher nodes, will move into the teacher node and cover them. This is true for both structured data that corresponds to small teacher networks with few intermediate nodes, or noisy/random data that correspond to large teachers with many intermediate nodes. This explains why the same network can fit both structured and random data (Fig. 2(a-b)).

Over-parameterization. In over-parameterization, lots of student nodes are initialized randomly at each layer. Any teacher node is more likely to have a substantial overlap with some student nodes, which leads to fast convergence (Fig. 2(a) and (c), Thm. 4), consistent with (6; 7). This also explains that training models whose capacity just fit the data (or teacher) yields worse performance (19).

Flat minima. Deep networks often converge to “flat minima” whose Hessian has a lot of small eigenvalues (28; 29; 21; 2). Furthermore, while controversial (4), flat minima seem to be associated with good generalization, while sharp minima often lead to poor generalization (12; 14; 36; 20). In our theory, when fitting with structured data, only a few lucky student nodes converge to the teacher, while for other nodes, their fan-out weights shrink towards zero, making them (and their fan-in weights) irrelevant to the final outcome (Thm. 5), yielding flat minima in which movement along most dimensions (“unlucky nodes”) results in minimal change in output. On the other hand, sharp min-
Structured Data (Small teacher network)  
Weight Initialization  
Convergence  
The Effect of over-parameterization  
Random Data (large teacher network)  
Weight Initialization  
Convergence  

Figure 1. (a) Teacher-Student Setting. For each node $j$, the activation region is $E_j = \{x : f_j(x) > 0\}$. (b) node $j$ initialized to overlap substantially with a teacher node $j^t$ converges faster towards $j^t$ (Thm. 4). (c) Student nodes initialized to be close to teacher converges to them, while the fan-out weights of other irrelevant student nodes go to zero. (Thm. 5).

Over-parameterization can still handle them and achieves zero training error.

Figure 2. Explanation of implicit regularization. Blue are activation regions of teacher nodes, while orange are students’. (a) When the data labels are structured, the underlying teacher network is small and each layer has few nodes. Over-parameterization (lots of red regions) covers them all. Moreover, those student nodes that heavily overlap with the teacher nodes converge faster (Thm. 4), yield good generalization performance. (b) If a dataset contains random labels, the underlying teacher network that can fit to it has a lot of nodes. Over-parameterization can still handle them and achieves zero training error.

Figure 3. Explanation of lottery ticket phenomenon. (a) A successful training with over-parameterization (2 filters in the teacher network and 4 filters in the student network). Node $j_3$ and $j_4$ are lucky draws with strong overlap with two teacher node $j^t_1$ and $j^t_2$, and thus converges with high weight magnitude. (b) Lottery ticket phenomenon: initialize node $j_3$ and $j_4$ with the same initial weight, clamp the weight of $j_1$ and $j_2$ to zero, and retrain the model, the test performance becomes better since $j_3$ and $j_4$ still converge to their teacher node, respectively. (c) If we reinitialize node $j_3$ and $j_4$, it is highly likely that they are not overlapping with teacher node $j^t_1$ and $j^t_2$ so the performance is not good.

Implicit regularization. On the other hand, the snapping behavior enforces winner-take-all: after optimization, a teacher node is fully covered (explained) by a few student nodes, rather than splitting amongst student nodes due to over-parameterization. This explains why the same network, once trained with structured data, can generalize to the test set.

Lottery Tickets. Lottery Tickets (6; 7) is an interesting phenomenon: if we reset “salient weights” (trained weights with large magnitude) back to the values before optimization but after initialization, prune other weights (often $> 90\%$ of total weights) and retrain the model, the test performance is the same or better; if we reinitialize salient weights, the test performance is much worse. In our theory, the salient weights are those lucky regions ($E_{j_3}$ and $E_{j_4}$ in Fig. 3) that happen to overlap with some teacher nodes after initialization and converge to them in optimization. Therefore, if we reset their weights and prune others away, they can still converge to the same set of teacher nodes, and potentially achieve better performance due to less interference with other irrelevant nodes. However, if we reinitialize them, they are likely to fall into unfavorable regions which cannot cover teacher nodes, and therefore lead to poor performance (Fig. 3(c)), just like in the case of under-parameterization.

2. Overview of the Framework

The details of our proposed theory can be found in Appendix (Sec. 5). Here we list the summary. First we show that for multilayered ReLU, there exists a relationship between the gradient $g_j(x)$ of a student node $j$ and teacher and student’s activations of the same layer (Thm. 1):

$$g_j(x) = f_j^t(x) \left[ \sum_j \beta_{j^tj}(x) f_j^t(x) - \sum_{j'} \beta_{j^tj'}(x) f_{j'}(x) \right],$$

where $f_j^t$ is the activation of node $j^t$ in the teacher, and $j'$ is the node at the same layer in the student. For each node $j$, we don’t know which teacher node corresponds to it, hence the linear combination terms. Typically the number of student nodes is much more than that of teachers’.

Thm. 1 applies to arbitrarily deep ReLU networks.

Then with a mild assumption (Assumption 1), we can write the gradient update rule of each layer $l$ in the following...
concise form (also Eqn. 8 in the Appendix):
\[ W_\ell = L_\ell W_\ell^* H_{\ell-1}^* - L_\ell W_\ell H_{\ell-1} \quad (2) \]
where \( L \) and \( L^* \) are correlations matrix of activations from the bottom layers, and \( H \) and \( H^* \) are modulation matrix from the top layers.

We then make an assumption that different teacher nodes of the same layer have small overlap in node activations (Assumption 3 and Fig. 7), and verify it in VGG16/VGG11 by showing that the majority of their BatchNorm bias are negative (Fig. 4 and Fig. 14). With this assumption, we prove two theorems:

- When the number of student nodes is the same as the number of teacher nodes \( (m_l = n_l) \), and each student’s weight vector \( w_j \) is close to a corresponding teacher \( w_j^* \), then the dynamics of Eqn. 2 yields (recovery) convergence \( w_j \rightarrow w_j^* \) (Thm. 4). Furthermore, such convergence is super-linear (i.e., the convergence rate is higher when the weights are closer).

- In the over-parameterization setting \( (m_l > n_l) \), we show that in the 2-layer case, with the help of top-layer, the portion of weights \( W_u \) that are close to teacher \( W^* \) converge \( (W_u \rightarrow W^*) \). For other irrelevant weights, while their final values heavily depends on initialization, with the help of top-down modulation, their fan-out top-layer weights converge to zero, and thus have no influence on the network output.

3. Experiments

3.1. Checking Assumption 3

To make Theorem 4 and Theorem 5 work, we make Assumption 3 that the activation field of different teacher nodes should be well-separated. To justify this, we analyze the BatchNorm bias of pre-trained VGG11 and VGG16. We check the BatchNorm bias \( c_1 \) as both VGG11 and VGG16 use Linear-BatchNorm-ReLU architecture. After BatchNorm first normalizes the input data into zero mean distribution, the BatchNorm bias determines how much data pass the ReLU threshold. If the bias is negative, then a small portion of data pass ReLU gating and Assumption 3 is likely to hold. From Fig. 4, it is quite clear that the majority of BatchNorm bias parameters are negative, in particular for the top layers.

3.2. Experiment Setup

We evaluate both the fully connected (FC) and ConvNet setting. For FC, we use a ReLU teacher network of size 50-75-100-125. For ConvNet, we use a teacher with channel size 64-64-64-64. The student networks have the same depth but with 10x more nodes/channels at each layer, such that they are substantially over-parameterized. When BatchNorm is added, it is added after ReLU.

We use random i.i.d Gaussian inputs with mean 0 and std 10 (abbreviated as GAUS) and CIFAR-10 as our dataset in the experiments. GAUS generates infinite number of samples while CIFAR-10 is a finite dataset. For GAUS, we use a random teacher network as the label provider (with 100 classes). To make sure the weights of the teacher are weakly overlapped, we sample each entry of \( w_j^* \) from \([-0.5, -0.25, 0, 0.25, 0.5]\), making sure they are non-zero and mutually different within the same layer, and sample biases from \( U[-0.5, 0.5] \). In the FC case, the data dimension is 20 while in the ConvNet case it is \( 16 \times 16 \). For CIFAR-10 we use a pre-trained teacher network with BatchNorm. In the FC case, it has an accuracy of 54.95%; for ConvNet, the accuracy is 86.4%. We repeat 5 times for all experiments, with different random seed and report min/max values.

Two metrics are used to check our prediction that some lucky student nodes converge to the teacher:

- Normalized correlation \( \bar{\rho} \). We compute normalized correlation (or cosine similarity) \( \rho \) between teacher and student activations evaluated on a validation set. At each layer, we average the best correlation over teacher nodes: \( \bar{\rho} = \text{mean}_j \text{max}_j \rho_{jj^*} \), where \( \rho_{jj^*} \) is computed for each teacher and student pairs \((j, j^*)\). \( \bar{\rho} \approx 1 \) means that most teacher nodes are covered by at least one student.

- Mean Rank \( \bar{r} \). After training, each teacher node \( j^* \) has the most correlated student node \( j \). We check the correlation rank of \( j \), normalized to \([0, 1]\) (0=rank first), back at initialization and at different epoches, and average them over teacher nodes to yield mean rank \( \bar{r} \). Small \( \bar{r} \) means that student nodes that initially correlate well with the teacher keeps the lead toward the end of training.

3.3. Results

Experiments are summarized in Fig. 5 and Fig. 6. \( \bar{\rho} \) indeed grows during training, in particular for low layers that are closer to the input, where \( \bar{\rho} \) moves towards 1. Furthermore, the final winning student nodes also have a good rank at the early stage of training. BatchNorm helps a lot, in particular for the CNN case with GAUS dataset. For CIFAR-10, the final evaluation accuracy (see Appendix) learned by the student is often \( \sim 1\% \) higher than the teacher. Using BatchNorm accelerates the growth of accuracy, improves \( \bar{r} \), but seems not to accelerate the growth of \( \bar{\rho} \).

The theory also predicts that the top-down modulation \( \beta \) helps the convergence. For this, we plot \( \beta_{jj^*} \) at different layers during optimization on GAUS. For better visualization, we align each student node index \( j \) with a teacher node \( j^* \) according to highest \( \rho \). Despite the fact that correlations are computed from the low-layer weights, it matches well with the top-layer modulation (identity matrix structure in Fig. 16). More ablation studies are in Sec. 8.

4. Conclusion

We propose a novel mathematical framework for multi-layered ReLU networks. This could tentatively explain many puzzling empirical phenomena in deep learning.
Figure 4. Distribution of BatchNorm bias in pre-trained VGG16 on ImageNet. Orange/blue are positive/negative biases. The first plot corresponds to the lowest layer (closest to the input). VGG11 in Fig. 14.

Figure 5. Correlation $\rho$ and mean rank $\bar{r}$ over training on GAUS. $\rho$ steadily grows and $\bar{r}$ quickly improves over time. Layer-0 (the lowest layer that is closest to the input) shows best match with teacher nodes and best mean rank. BatchNorm helps achieve both better correlation and lower $\bar{r}$, in particular for the CNN case.

Figure 6. Same experiment setting as in Fig. 5 on CIFAR-10. BatchNorm helps achieve lower $\bar{r}$. 
References


5. Appendix: Mathematical Framework

**Notation.** Consider a student network and its associated teacher network (Fig. 1(a)). Denote the input as \( x \). For each node \( j \), denote \( f_j(x) \) as the activation, \( f'_j(x) \) as the ReLU gating, and \( g_j(x) \) as the backpropagated gradient, all as functions of \( x \). We use the superscript \( \circ \) to represent a teacher node (e.g., \( j^\circ \)). Therefore, \( g_j \) never appears as teacher nodes are not updated. We use \( w_{jk} \) to represent weight between node \( j \) and \( k \) in the student network. Similarly, \( w'_{jk} \) represents the weight between node \( j^\circ \) and \( k^\circ \) in the teacher network.

We focus on multi-layered ReLU networks. We use the following equality extensively: \( \sigma(x) = \sigma'(x)x \). For ReLU node \( j \), we use \( E_j \equiv \{ x : f_j(x) > 0 \} \) as the activation region of node \( j \).

**Objective.** We assume that both the teacher and the student output probabilities over \( C \) classes. We use the output of teacher as the input of the student. At the top layer, each node \( c \) in the student corresponds to each node \( c^\circ \) in the teacher. Therefore, the objective is:

\[
\min_w J(w) = \frac{1}{2} \mathbb{E}_x [||f_c(x) - f_{c^\circ}(x)||^2]
\]  

(3)

By the backpropagation rule, we know that for each sample \( x \), the (negative) gradient \( g_c(x) \equiv \partial J/\partial f_c = f_{c^\circ}(x) - f_c(x) \). The gradient gets backpropagated until the first layer is reached.

Note that here, the gradient \( g_c(x) \) sent to node \( c \) is **correlated** with the activation of the corresponding teacher node \( f_{c^\circ}(x) \) and other student nodes at the same layer. Intuitively, this means that the gradient “pushes” the student node \( c \) to align with class \( c^\circ \) of the teacher. If so, then the student learns the corresponding class well. A natural question arises:

*Are student nodes at intermediate layers correlated with teacher nodes at the same layers?*

One might wonder this is hard since the student’s intermediate layer receives no **direct supervision** from the corresponding teacher layer, but relies only on backpropagated gradient. Surprisingly, the following theorem shows that it is possible for every intermediate layer:

**Theorem 1** (Recursive Gradient Rule). *If all nodes \( j \) at layer \( l \) satisfies Eqn. 4*

\[
g_j(x) = f'_j(x) \left[ \sum_{j'} \beta_{jj'} (x)f_{j'}(x) - \sum_{j'} \beta_{jj'} (x)f_{j'}(x) \right],
\]

(4)

then all nodes \( k \) at layer \( l - 1 \) also satisfies Eqn. 4 with \( \beta_{kk'} (x) \) and \( \beta_{kk'} (x) \) defined as follows:

\[
\beta_{kk'} (x) = \sum_{jj'} w_{jk} f'_j(x) \beta_{jj'} (x) f_{j'}(x) w_{j'k'}, \quad \beta_{kk'} (x) = \sum_{jj'} w_{jk} f'_j(x) \beta_{jj'} (x) f_{j'}(x) w_{j'k'}
\]

(5)

Note that this formulation allows different number of nodes for the teacher and student. In particular, we consider the over-parameterization setting: the number of nodes on the student side is much larger (e.g., 5-10x) than the number of nodes on the teacher side. Using Theorem 1, we discover a novel and concise form of gradient update rule:

**Assumption 1** (Separation of Expectations).

\[
\mathbb{E}_x [\beta_{jj'} (x) f'_j(x) f_{j'}(x) f_k(x) f_{k'}(x)] = \mathbb{E}_x [\beta_{jj'} (x)] \mathbb{E}_x [f'_j(x) f_{j'}(x)] \mathbb{E}_x [f_k(x) f_{k'}(x)]
\]

(6)

\[
\mathbb{E}_x [\beta_{jj'} (x) f'_j(x) f_{j'}(x) f_k(x) f_{k'}(x)] = \mathbb{E}_x [\beta_{jj'} (x)] \mathbb{E}_x [f'_j(x) f_{j'}(x)] \mathbb{E}_x [f_k(x) f_{k'}(x)]
\]

(7)

**Theorem 2.** *If Assumption 1 holds, the gradient dynamics of deep ReLU networks with objective (Eqn. 3) is:*

\[
\dot{W}_l = L_l^* W_l^* H_{l+1}^* - L_l W_l H_{l+1}
\]

(8)

Here we explain the notations. \( W_l^* = [w_{1l}^*, \ldots, w_{nl}^*] \) is \( n_l \) teacher weights, \( \beta_{l+1}^* = \mathbb{E}_x [\beta_{jj'} (x)] \), \( d_{jj'}^* = \mathbb{E}_x [f'_j(x) f_{j'}(x)] \) and \( D_l^* = [d_{jj'}^*] \). At the lowest layer \( l = 0 \), \( L_0 = \Delta_0 \), at the highest layer \( l = l_{max} - 1 \) where there is no ReLU, we have \( \beta_{max}^* = \beta_{max}^* = H_{max}^* = H_{max}^* = I \). We can define similar notations for \( W \) (which has \( n_l \) columns/filters), \( \beta \), \( D \), \( H \) and \( L \) (Fig. 7(c)). At the lowest layer \( l = 0 \), \( L_0 = \Delta_0 \), at the highest layer \( l = l_{max} - 1 \) where there is no ReLU, we have \( \beta_{max}^* = \beta_{max}^* = H_{max}^* = H_{max}^* = I \).
6. Appendix: Analysis on the Dynamics

In the following, we will use Eqn. 8 to analyze the dynamics of the multi-layer ReLU networks. For convenience, we first define the two functions \( \psi_l \) and \( \psi_d \) (\( \sigma \) is the ReLU function):

\[
\psi_l(w, w') = \mathbb{E}_x \left[ \sigma(w^T x) \sigma(w'^T x) \right], \quad \psi_d(w, w') = \mathbb{E}_x \left[ \|w^T x\| I(w'^T x) \right].
\]

We assume these two functions have the following property:

**Assumption 2** (Lipschitz condition). There exists \( K_d \) and \( K_l \) so that:

\[
\|\psi_i(w_1, w_2) - \psi_i(w_i, w_2)\| \leq \psi_i(w_1, w_1)(1 + K_i\|w_i - w_2\|), \quad i \in \{d, l\}
\]

Using this, we know that \( d_{ij} = \psi_d(w_j, w_j') \), \( d_{ij}^* = \psi_d(w_j, w_j^*) \), and so on. For brevity, denote \( d_{ij}^* = \psi_d(w_j^*, w_j^*) \) (when notation \( j_i^* \) is heavy) and so on. We impose the following assumption:

**Assumption 3** (Small Overlap between teacher nodes). There exists \( \epsilon_i \ll 1 \) and \( \epsilon_d \ll 1 \) so that:

\[
d_{ij2}^* \leq \epsilon_d d_{ij1}^*, \quad l_{ij2}^* \leq \epsilon_i l_{ij1}^* (\text{or } \epsilon_l l_{ij2}^*), \quad \text{for } j_1 \neq j_2.
\]

Intuitively, this means that the probability of the simultaneous activation of two teacher nodes \( j_1 \) and \( j_2 \) is small. One such case is that the teacher has negative bias, which means that they cut corners in the input space (Fig. 7a). We have empirically verified that the majority of biases in BatchNorm layers (after the data are whitened) are negative in VGG11/16 trained on ImageNet (Sec. 3.1).

6.1. Effects of BatchNorm

Batch Normalization (13) has been extensively used to speed up the training, reduce the tuning efforts and improve the test performance of neural networks. Here we use an interesting property of BatchNorm: the total “energy” of the incoming weights of each node \( j \) is conserved over training iterations:

**Theorem 3** (Conserved Quantity in Batch Normalization). For Linear \( \rightarrow \) ReLU \( \rightarrow \) BN or Linear \( \rightarrow \) BN \( \rightarrow \) ReLU configuration, \( \|w_j\| \) of a filter \( j \) before BN remains constant in training. (Fig. 11).

See Appendix for the proof. This may partially explain why BN has stabilization effect: energy will not leak from one layer to nearby ones. Due to this property, in the following, for convenience we assume \( \|w_j\|^2 = \|w_j^*\|^2 = 1 \), and the gradient \( \dot{w}_j \) is always orthogonal to the current weight \( w_j \). Note that on the teacher side we can always push the magnitude component to the upper layer; on the student side, random initialization naturally leads to constant magnitude of weights.

6.2. Same number of student nodes as teacher

If \( n_i = m_i \), \( L_i^* = L_i = I \) (e.g., the input of layer \( l \) is whitened) and \( \beta_{l+1}^* = \beta_{l+1} = 11^T \) (all \( \beta \) entries are 1), then the following theorem shows that weight recovery could follow (we use \( j' \) as \( j^* \)).

**Theorem 4.** For dynamics \( \dot{w}_j = P_{w_j}^+(W^* h_j^* - Wh_j) \), where \( P_{w_j}^+ \equiv I - w_j w_j^T \) is a projection matrix into the orthogonal complement of \( w_j \), \( h_j^* \) and \( h_j \) are corresponding \( j \)-th column in \( H^* \) and \( H \). Denote \( \theta_j = \angle(w_j, w_j^*) \) and assume \( \theta_j \leq \theta_0 \). If \( \gamma = \cos \theta_0 - (m-1)\epsilon_d M_d > 0 \), then \( \dot{w}_j \rightarrow w_j^* \) with the rate \( 1 - \eta d^* \) (\( \eta \) is learning rate). Here \( d = [1 + 2K_d \sin(\theta_0/2)] \min_j d_{jj}^0 \) and \( M_d = (1 + K_d) [1 + 2K_d \sin(\theta_0/2)]^2 / \cos \theta_0 \).
For simplicity, the theorem uses a uniform (and conservative) Accelerated convergence and learning rate schedule.

Pruning small weights in magnitude (8; 6) and pruning weights suggested by Hessian (18; 9). It also suggests a principled understanding of pruning methods could explain why there are many flat directions in trained networks, and why many eigenvalues of the Hessian are close to zero.

6.3. Over-Parameterization and Top-down Modulation

In the over-parameterization case ($n_t > m_t$, e.g., 5-10x), we arrange the variables into two parts: $W = [W_u, W_r]$, where $W_u$ contains $m_t$ columns (same size as $W^*$), while $W_r$ contains $n_t - m_t$ columns. We use $[u]$ (or $u$-set) to specify nodes $1 \leq j \leq m$, and $[r]$ (or $r$-set) for the remaining part.

In this case, if we want to show “the main component” $W_u$ converges to $W^*$, we will meet with one core question: to where will $W_r$ converge, or whether $W_r$ will even converge at all? We need to consider not only the dynamics of the current layer, but also the dynamics of the upper layer. Using a 1-hidden layer over-parameterized ReLU network as an example, Theorem 5 shows that the upper-layer dynamics $\dot{V} = L^*V^* - LV$ automatically apply top-down modulation to suppress the influence of $W_r$, regardless of their convergence. Here $V = \begin{bmatrix} V_u \\ V_r \end{bmatrix}$, where $V_u$ are the weight components of $u$-set. See Fig. 8.

Theorem 5 (Over-Parameterization and Top-down Modulation). Consider $\dot{W} = W^*H^* - WH$ with over-parameterization ($n > m$) and its upper-layer dynamics $\dot{V} = L^*V^* - LV$. Assume that initial value $W_0$ is close to $W^*$: $\theta_j = \angle(w_j, w_j^*) \leq \theta_0$ for $j \in [u]$. If (1) Assumption 3 holds for all pairwise combination of columns of $W^*$ and $W^0$, and (2) there exists $\gamma = \gamma(\theta_0, m) > 0$ and $\bar{\lambda}$ so that Eqn. 43 and Eqn. 44 holds, then $W_u \to W^*$, $V_u \to V^*$ and $V_r \to 0$ with rate $1 - \eta\bar{\lambda}$. See Appendix for the proof (and definition of $\bar{\lambda}$ in Eqn. 47). The intuition is: if $W_u$ is close to $W^*$ and $W_r$ are far away from them due to Assumption 3, the off-diagonal elements of $L$ and $L^*$ are smaller than diagonal ones. This causes $V_u$ to move towards $V^*$ and $V_r$ to move towards zero. When $V_r$ becomes small, so does $\beta_j$ for $j \in [r]$ or $j' \in [r]$. This in turn supresses the effect of $W_r$ and accelerates the convergence of $W_u$. $V_r \to 0$ exponentially so that $W_r$ stays close to its initial locations, and Assumption 3 holds for all iterations. A few remarks:

Flat minima. Since $V_r \to 0$, $W_r$ can be changed arbitrarily without affecting the outputs of the neural network. This could explain why there are many flat directions in trained networks, and why many eigenvalues of the Hessian are close to zero.

Understanding of pruning methods. Theorem 5 naturally relates two different unstructured network pruning approaches: pruning small weights in magnitude (8; 6) and pruning weights suggested by Hessian (18; 9). It also suggests a principled structured pruning method: instead of pruning a filter by checking its weight norm, pruning accordingly to its top-down modulation.

Accelerated convergence and learning rate schedule. For simplicity, the theorem uses a uniform (and conservative)
\( \gamma \) throughout the iterations. In practice, \( \gamma \) is initially small (due to noise introduced by \( r \)-set) but will be large after a few iterations when \( V_r \) vanishes. Given the same learning rate, this leads to accelerated convergence. At some point, the learning rate \( \eta \) becomes too large, leading to fluctuation. In this case, \( \eta \) needs to be reduced.

**Many-to-one mapping.** Theorem 5 shows that under strict conditions, there is one-to-one correspondence between teacher and student nodes. In general this is not the case. Two students nodes can be both in the vicinity of a teacher node \( w^*_j \) and converge towards it, until that node is fully explained. We leave it to the future work for rigid mathematical analysis of many-to-one mappings.

**Random initialization.** One nice thing about Theorem 5 is that it only requires the initial \( \|W_u - W^*\| \) to be small. In contrast, there is no requirement for small \( \|V_r\| \). Therefore, we could expect that with more over-parameterization and random initialization, in each layer \( l \), it is more likely to find the \( w \)-set (of fixed size \( m_l \)), or the lucky weights, so that \( W_u \) is quite close to \( W^* \). At the same time, we don’t need to worry about \( \|W_r\| \) which grows with more over-parameterization. Moreover, random initialization often gives orthogonal weight vectors, which naturally leads to Assumption 3.

**6.4. Extension to Multi-layer ReLU networks**

Using a similar approach, we could extend this analysis to multi-layer cases. We conjecture that similar behaviors happen: for each layer, due to over-parameterization, the weights of some lucky student nodes are close to the teacher ones. While these converge to the teacher, the final values of others irrelevant weights are initialization-dependent. If the irrelevant nodes connect to lucky nodes at the upper-layer, then similar to Thm. 5, the corresponding fan-out weights converge to zero. On the other hand, if they connect to nodes that are also irrelevant, then these fan-out weights are not-determined and their final values depends on initialization. However, it doesn’t matter since these upper-layer irrelevant nodes eventually meet with zero weights if going up recursively, since the top-most output layer has no over-parameterization. We leave a formal analysis to future work.

**7. Appendix: Proofs**

**7.1. Theorem 1**

*Proof.* The first part of gradient backpropagated to node \( j \) is:

\[
g^*_j(x) = f^*_j(x) \sum_{j^o} \beta^*_j(x) f^*_j(x)
\]

\[
g^*_j(x) = f^*_j(x) \sum_{j^o} \beta^*_j(x) f^*_j(x) \sum_{k^o} w^*_j k^o f^*_k(x)
\]

\[
g^*_j(x) = \sum_{k^o} \left[ f^*_j(x) \sum_{j^o} \beta^*_j(x) f^*_j(x) w^*_j k^o \right] f^*_k(x)
\]
Therefore, for the gradient to node \( k \), we have:

\[
g_k(x) = f'_k(x) \sum_j w_{jk} g_j^1(x) = \sum_j \left[ \sum_{k^o} w_{jk} f'_j(x) \beta_{kj^o}^\ast(x) f_{k^o}(x) \right] f_k(x)
\]

(15)

\[
g_k(x) = f'_k(x) \sum_{k^o} \sum_j w_{jk} f'_j(x) \beta_{kj^o}^\ast(x) f_{k^o}(x) w_{j^o k^o}^\ast \beta_{j^o k^o}^\ast(x)
\]

(16)

And similar for \( \beta_{kk'}(x) \). Therefore, by mathematical induction, we know that all gradient at nodes in different layer follows the same form. \( \square \)

### 7.2. Theorem 2

**Proof.** Using Thm. 1, we can write down weight update for weight \( w_{jk} \) that connects node \( j \) and node \( k \):

\[
\hat{w}_{jk} = \sum_{j^o, k^o} w_{j^o k^o}^\ast \frac{\mathbb{E}_x \left[ f'_j(x) \beta_{j^o j^o}^\ast(x) f_{j^o}(x) f_{k^o}(x) \right]}{\beta_{j^o k^o}^\ast} - \sum_{j', k'} w_{j' k'} \mathbb{E}_x \left[ f'_j(x) \beta_{j' j'}(x) f_{j'}(x) f_{k'}(x) \right] \beta_{j' k'}^\ast
\]

(17)

Note that \( j^o, k^o, j' \) and \( k' \) run over all parents and children nodes on the teacher side. This formulation works for over-parameterization (e.g., \( j^o \) and \( j' \) can run over different nodes). Applying Assumption 1 and rearrange terms in matrix form yields Eqn. 8. \( \square \)

### 7.3. Theorem 3

**Proof.** Given a batch with size \( N \), denote pre-batchnorm activations as \( f = [f_j(x_1), \ldots, f_j(x_N)]^T \) and gradients as \( g = [g_j(x_1), \ldots, g_j(x_N)]^T \) (See Fig. 10(a)). \( \tilde{f} = (f - \mu)/\sigma \) is its whitened version, and \( c_0\tilde{f} + c_1 \) is the final output of BN. Here \( \mu = \frac{1}{N} \sum_i f_j(x_i) \) and \( \sigma^2 = \frac{1}{N} \sum_i (f_j(x_i) - \mu)^2 \) and \( c_1, c_0 \) are learnable parameters. With vector notation, the gradient update in BN has a compact form with clear geometric meaning:

**Lemma 1** (Backpropagation of Batch Norm (34)). For a top-down gradient \( g \), BN layer gives the following gradient update (\( P^L_{11} \) is the orthogonal complementary projection of subspace \( \{ f, 1 \} \)):

\[
g_f = J^N_B(f)g = \frac{c_0}{\sigma} P^L_{11}g, \quad g_c = S(f)^T g
\]

(18)
Intuitively, the back-propagated gradient $J^{BN}(f)g$ is zero-mean and perpendicular to the input activation $f$ of BN layer, as illustrated in Fig. 10. Unlike (15; 37) that analyzes BN in an approximate manner, in Thm. 1 we do not impose any assumptions.

Given Lemma 1, we can prove Thm. 3. For Fig. 11(a), using the property that $E_x[f_j^{lin}g_j^{lin}] = 0$ (the expectation is taken over batch) and the weight update rule $w_{jk} = E_x[f_j^{lin}f_k]$ (over the same batch), we have:

$$\frac{1}{2} \frac{d}{dt} \|w_j\|^2 = \sum_{k \in ch(j)} w_{jk} \dot{w}_j = E_x \left[ \sum_{k \in ch(j)} w_{jk} f_k(x) g_j^{lin}(x) \right] = E_x \left[ f_j^{lin}(x) g_j^{lin}(x) \right] = 0 \quad (19)$$

For Fig. 11(b), note that $E_x[g_j^{lin}f_j^{lin}] = E_x[g_j^{rl}f_j^{rl}] = E_x[g_j^{rl}f_j^{rl}] = 0$ and conclusion follows.

$$\square$$

7.4. Lemmas

For simplicity, in the following, we use $\delta w_j = w_j - w_j^*$.

**Lemma 2** (Bottom Bounds). Assume all $\|w_j\| = \|w_{j'}\| = 1$. Denote

$$p_{j,j'}^* \equiv w_j^*d_{j,j'}^*, \quad p_{j,j'} \equiv w_{j'}d_{j,j'}^*, \quad \Delta p_{j,j'}^* \equiv p_{j,j'}^* - p_{j,j'}$$

If Assumption 2 holds, we have:

$$\|\Delta p_{j,j'}\| \leq (1 + K_d)\|\delta w_{j'}\| \quad (20)$$

If Assumption 3 also holds, then:

$$d_{j,j'}^* \leq \epsilon_d(1 + K_d\|\delta w_{j'}\|)(1 + K_d\|\delta w_{j'}\|)d_{j,j'}^* \quad (21)$$

**Proof.** We have for $j \neq j'$:

$$\|\Delta p_{j,j'}\| = \|w_j^*d_{j,j'}^* - w_{j'}d_{j,j'}^*\| \leq \|w_j^*(d_{j,j'}^* - d_{j,j'}^*) + (w_{j'} - w_j^*)d_{j,j'}^*\| \leq \|w_j^*\|\|d_{j,j'}^* - d_{j,j'}^*\| + \|w_{j'} - w_j^*\|\|d_{j,j'}^*\| \leq d_{j,j'}^*K_d\|\delta w_{j'}\| + d_{j,j'}^*\|\delta w_{j'}\| \leq (1 + K_d)d_{j,j'}^*\|\delta w_{j'}\| \quad (22)$$

If Assumption 3 also holds, we have:

$$d_{j,j'}^* \leq d_{j,j'}^*(1 + K_d\|\delta w_{j'}\|) \leq \epsilon_d d_{j,j'}^*(1 + K_d\|\delta w_{j'}\|) \leq \epsilon_d d_{j,j'}^*(1 + K_d\|\delta w_{j'}\|)(1 + K_d\|\delta w_{j'}\|) \quad (23)$$

$$\square$$

**Lemma 3** (Top Bounds). Denote

$$q_{j,j'}^* \equiv v_j^*l_{j,j'}^*, \quad q_{j,j'} \equiv v_{j'}l_{j,j'}^*, \quad \Delta q_{j,j'} \equiv q_{j,j'}^* - q_{j,j'}$$

If Assumption 2 holds, we have:

$$\|\Delta q_{j,j'}\| \leq (1 + K_i)l_{j,j'}^*\|\delta w_{j'}\| \quad (24)$$

If Assumption 3 also holds, then:

$$l_{j,j'}^* \leq \epsilon_t(1 + K_i\|\delta w_{j'}\|)(1 + K_i\|\delta w_{j'}\|)l_{j,j'}^* \quad (25)$$

**Proof.** The proof is similar to Lemma 2.

$$\square$$

**Lemma 4** (Quadratic fall-off for diagonal elements of $L$). For node $j$, we have:

$$\|l_{jj}^* - l_{jj}\| \leq C_0 l_{jj}^*\|\delta w_{j}\|^2 \quad (26)$$

**Proof.** The intuition here is that both the volume of the affected area and the weight difference are proportional to $\|\delta w_{j}\|$. $\|l_{jj}^* - l_{jj}\|$ is their product and thus proportional to $\|\delta w_{j}\|^2$. See Fig. 12.

$$\square$$
Since \(\|\delta w_j\| = 2 \sin \frac{\theta}{2} \leq 2 \sin \frac{\theta_0}{2}\). So given \(\theta_0\), we also have a bound for \(\|\delta w_j\|\).

When \(\beta = \beta^* = 11^2\), the matrix form can be written as the following:

\[
\delta w_j = w_j^* - w_j^+ = P_{w_j}^+ w_j h_j^* + \sum_{j' \neq j} P_{w_j}^+ (w_{j'}^* h_{j'}^* - w_{j'} h_{j'}^*) = P_{w_j}^+ p_j^+ + \sum_{j' \neq j} P_{w_j}^+ \Delta p_{j'}
\]

(35)

by using \(P_{w_j}^+ w_j = 0\) (and thus \(h_{j,j}\) doesn’t matter). Since \(\|w_j\|\) is conserved, it suffices to check whether the projected weight vector \(P_{w_j}^+ w_j\) of \(w_j\) onto the complementary space of the ground truth node \(w_j^*\) goes to zero:

\[
P_{w_j}^+ w_j = P_{w_j}^+ P_{w_j} w_j^* + \sum_{j' \neq j} P_{w_j}^+ P_{w_j} \Delta p_{j'}
\]

(36)

Denote \(\theta_j = \angle(w_j, w_j^*)\) and a simple calculation gives that \(\sin \theta_j = \|P_{w_j}^+ w_j\|\). First we have:

\[
P_{w_j}^+ P_{w_j} w_j^* = P_{w_j}^+ (I - w_j w_j^T) w_j^* = -P_{w_j}^+ w_j w_j^T w_j^* = -\cos \theta_j P_{w_j}^+ w_j
\]

(37)

From Lemma 2, we know that

\[
\|\Delta p_{j,j}\| \leq (1 + K_d)\|\delta w_j\| \leq \epsilon_d (1 + K_d) [1 + 2K_d \sin(\theta_0/2)]^2 \|\delta w_j\|
\]

(38)

Note that here we have \(\|\delta w_j\| = 2 \sin \frac{\theta}{2} = \sin \theta_j / \cos \frac{\theta}{2} \leq \sin \theta_j / \cos \frac{\theta_0}{2}\). We discuss finite step with very small learning rate \(\eta > 0\):

\[
\sin \theta_j^{t+1} = \|P_{w_j}^+ w_j^{t+1}\| = \|P_{w_j}^+ w_j^t + \eta P_{w_j}^+ \dot{w}_j^t\| \leq (1 - \eta d_{j,j}^* \cos \theta_j^t) \sin \theta_j^t + \eta d_{j,j} \sum_{j' \neq j} d_{j,j'}^* \sin \theta_j^{t+1}
\]

(39)

(40)

since \(\|P_{w_j}^+\| = \|P_{w_j}^+\| = 1\). Here

\[
M_d = (1 + K_d) [1 + 2K_d \sin(\theta_0/2)]^2 / \cos \frac{\theta_0}{2}
\]

(41)

is an iteration independent constant.

We set \(\gamma = \cos \theta_0 - (m-1)\epsilon_d M_d\). If \(\gamma > 0\), denote a constant \(\bar{d} = [1 + 2K_d \sin(\theta_0/2)] \min_j d_{j,j}^{t_0}\) and from Lemma 2 we know \(d_{j,j}^{t_0} \geq \bar{d}\) for all \(j\). Then given the inductive hypothesis that \(\sin \theta_j^t \leq (1 - \eta \bar{d} \gamma)^{t-1} \sin \theta_0\), we have:

\[
\sin \theta_j^{t+1} \leq (1 - \eta \bar{d} \gamma)^t \sin \theta_0
\]

(42)

Therefore, \(\sin \theta_j^t \to 0\), which means that \(w_j \to w_j^*\). □
A few remarks:

**The projection operator** $P_{\mathcal{W}_j}$. Note that $P_{\mathcal{W}_j}$ is important. Intuitively, without the projection, if the same proof logic worked, one could have concluded that $\mathbf{w}$ converges to any $\alpha \mathbf{w}^*$, where $\alpha$ is a constant scaling factor, which is obviously wrong.

Indeed, without $P_{\mathcal{W}_j}$, there would be a term $\mathbf{w}_j^* h_{jj}^* - \mathbf{w}_j h_{jj}$ on RHS. This term breaks into $\mathbf{w}_j(h_{jj}^* - h_{jj}) + (\mathbf{w}_j^* - \mathbf{w}_j)h_{jj}^*$. Although there could exist $C$ so that $\|h_{jj}^* - h_{jj}\| \leq C\|d\mathbf{w}_j\|$, unlike Lemma 4, $C$ may not be small, and convergence is not guaranteed.

7.6. Theorem 5

**Proof.** First, only for $j \in [u]$, we have their ground truth value $\mathbf{w}_j^*$. For $j \in [r]$, we assign $\mathbf{w}_j^* = \mathbf{w}_j^0$, i.e., their initial values. As we will see, this will make things easier.

From the assumption, we know that $\sin \theta_j \leq \sin \theta_0$ for $j \in [u]$. In addition, denote that $\|\delta \mathbf{v}_j^0\| \leq B_{\delta v}$ for $j \in [u]$. Denote $B_v$ as the bound for all $\|\mathbf{v}_j^0\|$.

Now suppose we can find a $\gamma > 0$ if the following set of equations are satisfied:

\[
\begin{align*}
\gamma &\geq (B_v - B_{\delta v}) \cos \theta_0 - \epsilon_d (B_v + B_{\delta v}) \max(B_{d,u}, B_{d,r}) > 0 \\
\gamma &\geq 1 - \epsilon_1 \max(B_{i,u}, B_{i,r}) - \kappa > 0
\end{align*}
\]

Here

\[
\begin{align*}
\bar{d} &= (1 - K_d C_{d,j}) \min_j d_{jj}^0 > 0 \\
\bar{l} &= (1 - K_l C_{l,j}) \min_j l_{jj}^0 > 0 \\
\bar{\lambda} &= \min(\bar{d}, \bar{l}) \\
\kappa &= 2C_0 \sin(\theta_0/2)(1 + B_{\delta v}) \\
C_{d,u} &= 2K_d \sin(\theta_0/2) \\
C_{d,r} &= \epsilon_d K_d \frac{B_{d,r}(B_v + B_{\delta v})B_v}{\lambda_\gamma(2 - \eta \lambda \gamma)} \\
M_{d}^{uu} &= (1 + K_d)(1 + C_{d,u})^2 / \cos \frac{\theta_0}{2} \\
M_{d}^{ur} &= (1 + K_d)(1 + C_{d,u})(1 + C_{d,r}) \\
M_{d}^{ru} &= (1 + K_d)(1 + C_{d,u}) / \cos \frac{\theta_0}{2} \\
M_{d}^{rr} &= (1 + K_d)(1 + C_{d,r})^2 \\
B_{d,u} &= (m - 1)M_{d}^{uu} + (n - m)M_{d}^{ur} \\
B_{d,r} &= (m - 1)M_{d}^{ru} + (n - m)M_{d}^{rr}
\end{align*}
\]

and similarly we can define $C_l$ and $M_l$ etc. If we can find such a $\gamma > 0$ then the dynamics converges. Here all $C$ are close to 0 and $M$ are close to 1.

Note that if $\epsilon_d$ and $\epsilon_1$ are small, it is obvious to see there exists a feasible $\gamma > 0$ (e.g., $\gamma = 1$).

To prove it, we maintain the following induction hypothesis for iteration $t$:

\[
\begin{align*}
d_{jj}^{tt} &\leq \epsilon_d M_{d,j,j'}d_{jj}^{tt}, \quad l_{jj}^{tt} &\leq \epsilon_l M_{l,j,j'}l_{jj}^{tt}, \quad j' \neq j \\
\sin \theta_j^t &\leq (1 - \eta \lambda \gamma)^{t-1} \sin \theta_0, \quad j \in [u] \\
\|\delta \mathbf{v}_j^t\| &\leq (1 - \eta \lambda \gamma)^{t-1} B_{\delta v}, \quad j \in [u], \quad \|\mathbf{v}_j^t\| &\leq (1 - \eta \lambda \gamma)^{t-1} B_v, \quad j \in [r]
\end{align*}
\]

Besides, the following condition is involved (but it is not part of induction hypothesis):

\[
\|\mathbf{w}_j^t - \mathbf{w}_j^0\| \leq C_{d,r}, \quad j \in [r]
\]
Now we discuss $j \in [u]$ and $j \in [r]$:

**Relevant nodes.** For $j \in [u]$, the first two terms are:

\[
\Delta q_{jj} = -l^{*}_{jj}\delta v_{j} + (l^{*}_{jj} - l_{jj})v_{j}
\]  

(61)

From Lemma 4 we know that:

\[
\|l^{*}_{jj} - l_{jj}\|v_{j}\| \leq C l^{*}_{jj}\|\delta w_{j}\|^2 \|v_{j}\| \leq 2C \sin(\theta_0/2)(1 + B_{\delta v})l^{*}_{jj}\|\delta w_{j}\| = \kappa l^{*}_{jj}\|\delta w_{j}\|
\]  

(62)
Since $\gamma$ satisfies Eqn. 44. 

**Irrelevant nodes.** Note that for $j \in [r]$, we don’t have the term $q_{jj}^*$. Therefore, we have:

$$
\|v_{j}^{t+1}\| \leq (1 - \eta l_{jj}^*)\|v_{j}^t\| + \eta l_{jj}^*\|v_{j}^t\| + \sum_{j' \neq j, j' \in [u]} \|v_{j'}^t\| + \sum_{j' \neq j, j' \in [r]} \|v_{j'}^t\|
$$

$$
\leq (1 - \eta l_{jj}^2)\|v_{j}^t\| + \eta l_{jj}^2\|v_{j}^t\| + \sum_{j' \neq j, j' \in [u]} \|v_{j'}^t\| + \sum_{j' \neq j, j' \in [r]} \|v_{j'}^t\|
$$

$$
\leq (1 - \eta l_{jj}^2)\|v_{j}^t\| + \eta l_{jj}^2\|v_{j}^t\| + \sum_{j' \neq j, j' \in [u]} \|v_{j'}^t\| + \sum_{j' \neq j, j' \in [r]} \|v_{j'}^t\|
$$

$$
\leq (1 - \eta l_{jj}^2)\|v_{j}^t\| + \eta l_{jj}^2\|v_{j}^t\| + \sum_{j' \neq j, j' \in [u]} \|v_{j'}^t\| + \sum_{j' \neq j, j' \in [r]} \|v_{j'}^t\|
$$

7.6.2. **Lemma 6**

**Proof.** Similar to the proof of Thm. 4, for node $j$, in the lower-layer, we have:

$$
\hat{w}_j = \sum_{j' \neq j} P_{w_j} \hat{p}_{jj'} + P_{w_j} \sum_{j' \in [u]} \Delta \hat{p}_{jj'} + P_{w_j} \sum_{j' \in [r]} \hat{p}_{jj'}
$$

where $h_{jj'} = d_{jj} v_j^T v_{j'}$. And $\hat{p}_{jj'} = p_{jj'} v_j^T v_{j'} = w_j h_{jj'}$.

Due to (W-Separation) and $\|w_{j'}\| = 1$, we know that for $j \neq j'$:

$$
\|\Delta \hat{p}_{jj'}\| \leq \epsilon_d d_{d,uu} d_{d,uu}^* \|\delta w_{j'}\| \|v_{j'}\|, \quad \|\hat{p}_{jj'}\| \leq \epsilon_d d_{d,uu} d_{d,uu}^* \|\delta w_{j'}\| \|v_{j'}\|, \quad j \in [u]
$$

$$
\|\Delta \hat{p}_{jj'}\| \leq \epsilon_d d_{d,rr} d_{d,rr}^* \|\delta w_{j'}\| \|v_{j'}\|, \quad \|\hat{p}_{jj'}\| \leq \epsilon_d d_{d,rr} d_{d,rr}^* \|\delta w_{j'}\| \|v_{j'}\|, \quad j \in [r]
$$

Note that if $\|v_{j'}\|$ (for $j \in [r]$) doesn’t converge to zero, then due to Eqn. 67, there is always residue and $w_j$ won’t converge to $w_j^*$.

Now we discuss two cases:

**Relevant nodes.** For $j \in [u]$, similar to Eqn. 37 we have:

$$
\sin \theta_j^{t+1} \leq (1 - \eta l_{jj}^2)\|v_{j}^t\| \|v_{j}^t\| \cos \theta_j^t + \eta \|v_{j}^t\| \|v_{j}^t\| \sin \theta_j^t + \sum_{j' \neq j, j \in [u]} \|v_{j'}^t\| \sin \theta_j^t + \sum_{j' \neq j} \|v_{j'}^t\|
$$

Since $(W_u$-Contraction) and $(V$-Contraction) holds for time $t$, we know that:

$$
\sin \theta_j^{t+1} \leq (1 - \eta l_{jj}^2)^{t+1} \sin \theta_0
$$

since Eqn. 43 holds.

**Irrelevant nodes.** In this case, we cannot prove for $j \in [r]$, $w_j$ converges to any determined target. Instead, we show that $w_j$ won’t move too much from its initial location $w_j^0$, which is also set to be $w_j^*$, before its corresponding $v_j$ converges to zero. This is important to ensure that (W-Separation) remains correct thorough-out the iterations.

For any $j \in [u]$, using $(W_u$-Contraction) and $(V$-Contraction), we know that the distance between the current $w_j$ and its
Figure 14. BatchNorm bias distribution of pre-trained VGG11 on ImageNet. Orange/blue are positive/negative biases. The first plot corresponds to the lowest layer (closest to the input).

\[ \| w^t_j - w^0_j \| \leq \eta \sum_{t'=0}^t \| \dot{w}^t_{j'} \| \leq \eta \sum_{t'=0}^t \| \Delta \bar{p}^t_{jj'} + \sum_{j' \in [r], j' \neq j} \bar{p}^t_{jj'} \| \]

\[ \leq \eta \epsilon_d B_{d,u} (B_v + B_{\beta v}) B_v \sum_{t'=0}^t (1 - \eta \lambda \gamma)^{2t'} \]

\[ = \frac{\epsilon_d B_{d,r} (B_v + B_{\beta v}) B_v}{\lambda \gamma (2 - \eta \lambda \gamma)} = C_{d,r} \]

Therefore, we prove that \((W_r\text{-Bound})\) holds for iteration \(t + 1\).

7.7. Lemma 7

Proof. Simply followed from combining Lemma 3, Lemma 2 and weight bounds \((W_u\text{-Contraction})\) and \((V\text{-Contraction})\).

8. Appendix: More experiments

Besides, we also perform ablation studies on GAUS.

**Size of teacher network.** As shown in Fig. 15(a), for small teacher networks (FC 10-15-20-25), the convergence is much faster and training without BatchNorm is faster than training with BatchNorm. For large teacher networks, BatchNorm definitely increases convergence speed and growth of \(\bar{\rho}\).

**Finite versus Infinite Dataset.** We also repeat the experiments with a pre-generated finite dataset of GAUS in the CNN case, and find that the convergence of node similarity stalls after a few iterations. This is because some nodes receive very few data points in their activated regions, which is not a problem for infinite dataset. We suspect that this is probably the reason why CIFAR-10, as a finite dataset, does not show similar behavior as GAUS.
Figure 15. Ablation studies on GAUS. (a) $\rho$ converges much faster in small models (10-15-20-25) than in large model (50-75-100-125). BatchNorm hurts in small models. (b) $\beta$ stalls using finite samples.

Figure 16. Visualization of (transpose of) $H^*$ and $\beta^*$ matrix before and after optimization (using GAUS). Student node indices are reordered according to teacher-student node correlations. After optimization, student node who has high correlation with the teacher node also has high $\beta$ entries. Such a behavior is more prominent in $H^*$ matrix that combines $\beta^*$ and the activation patterns $D^*$ of student nodes (Sec. 5).

Figure 17. Mean/Median rank at different epoch of the final winning student nodes that best match the teacher nodes after the training using BatchNorm. Gaussian (left) versus CIFAR10 (right). FC (top) versus CNN (bottom).
Figure 18. Mean/Median rank at different epoch of the final winning student nodes that best match the teacher nodes after the training without BatchNorm. Gaussian (left) versus CIFAR10 (right). FC (top) versus CNN (bottom).

Figure 19. Gaussian data with small (10-15-20-25) and large (50-75-100-125) FC models. Small models (top) versus large models (bottom). With BN (left) versus Without BN (right).

Figure 20. Gaussian CNN. With BN (top) versus Without BN (bottom). Finite Dataset (left) versus Infinite Dataset (right).