Good Subnetworks Provably Exist: Pruning via Greedy Forward Selection

Mao Ye 1 Chengyue Gong * 1 Lizhen Nie * 2 Denny Zhou 3 Adam Klivans 1 Qiang Liu 1

Abstract
Recent empirical works show that large deep neural networks are often highly redundant and one can find much smaller subnetworks without a significant drop of accuracy. However, most existing methods of network pruning are empirical and heuristic, leaving it open whether good subnetworks provably exist, how to find them efficiently, and if network pruning can be provably better than direct training using gradient descent. We answer these problems positively by proposing a simple greedy selection approach for finding good subnetworks, which starts from an empty network and greedily adds important neurons from the large network. This differs from the existing methods based on backward elimination, which remove redundant neurons from the large network. Theoretically, applying our greedy selection strategy on sufficiently large pre-trained networks guarantees to find small subnetworks with lower loss than networks directly trained with gradient descent. Practically, we improve prior arts of network pruning on learning compact neural architectures on ImageNet, including ResNet, MobilenetV2/V3, and ProxylessNet. Our theory and empirical results on MobileNet suggest that we should fine-tune the pruned subnetworks to leverage the information from the large model, instead of re-training from new random initialization as suggested in Liu et al. (2019b).

1. Introduction
The last few years have witnessed the remarkable success of large-scale deep neural networks (DNNs) in achieving human-level accuracy on complex cognitive tasks, including image classification (e.g., He et al., 2016), speech recognition (e.g., Amodei et al., 2016) and machine translation (e.g., Wu et al., 2016). However, the modern large-scale DNNs suffer from slow inference speed and high energy cost, which makes it difficult to deploy them on edge devices such as mobile phones and Internet of Things (IoT) (Cai et al., 2019). It is of increasing importance to obtain DNNs with small sizes and low energy costs.

Network pruning has been shown to be a successful approach for learning small and energy-efficient neural networks (e.g., Han et al., 2016b). These methods start with a pre-trained large neural network and remove the redundant units (neurons or filters/channels) to obtain a much smaller subnetwork without significant drop of accuracy. See e.g., Zhuang et al. (2018); Luo et al. (2017); Liu et al. (2017; 2019b); He et al. (2019; 2018b) for examples of recent works.

However, despite the recent empirical successes, thorough theoretical understandings on why and how network pruning works are still largely missing. Our work is motivated by the following basic questions:

The Subnetwork Problems: Given a pre-trained large (over-parameterized) neural network, does there exist a small subnetwork inside the large network that performs almost as well as the large network? How to find such a good subnetwork computationally efficiently? Does the small network pruned from the large network provably outperform the small network which has the same size but is directly trained from scratch?

We approach this problem by considering a simple greedy selection strategy, which starts from an empty network and constructs a good subnetwork by sequentially adding neurons from the pre-trained large network to yield the largest immediate decrease of the loss (see Figure 1(left)). This simple algorithm provides both strong theoretical guarantees and state-of-the-art empirical results, as summarized below:

Pruning Learns Good Subnetworks For two-layer neural networks, our analysis shows that our method yields a network of size $n$ with a loss of $O(1/n) + L_N^*$, where $L_N^*$ is the optimal loss we can achieve with all the neurons in the pre-trained large network of size $N$. Further, if the pre-trained large network is sufficiently over-parametrized, we
achieve a much smaller loss of $O(1/n^2)$. In comparison, standard training of networks of size $O(1/n^2)$ yields a loss of $O(1/n + \varepsilon)$ following the mean field analysis of Song et al. (2018); Mei et al. (2019), where $\varepsilon$ is usually a small term involving the loss of training infinitely wide networks. See Section 3.3 for more details.

Our fast $O(1/n^2)$ rate suggests that pruning from over-parameterized models guarantees to find more accurate small networks than direct training using gradient descent, providing a theoretical justification of the widely used network pruning paradigm.

Selection vs. Elimination Many of the existing methods of network pruning are based on backward elimination of the redundant neurons starting from the full large network, (e.g., Luo et al., 2017; Liu et al., 2017). In contrast, our method is based on forward selection, progressively growing the small network by adding the neurons; see Figure 1 for an illustration. Our empirical results show that, our forward selection achieves better accuracy on pruning DNNs under fixed FLOPs constraints, e.g., ResNet (He et al., 2016), MobileNetV2 (Sandler et al., 2018), ProxylessNet (Cai et al., 2019) and MobileNetV3 (Howard et al., 2019) on ImageNet. In particular, our method outperforms all prior arts on pruning MobileNetV2 on ImageNet. In particular, our method outperforms all prior arts on pruning MobileNetV2/MobileNetV3 gives much better performance than re-training it from a new random initialization, which violates the conclusions of Liu et al. (2019b). Besides, we observe that increasing the size of pre-trained large models yields better pruned subnetwork as predicted by our theory. See Section 4.2 and 4.3 for a thorough discussion.

Notation We use notation $[N] := \{1, \ldots, N\}$ for the set of the first $N$ positive integers. All the vector norms $\|\cdot\|$ are assumed to be $\ell_2$ norm. $\|\cdot\|_{\text{Lip}}$ and $\|\cdot\|_\infty$ denote Lipschitz and $\ell_\infty$ norm for functions. We denote $\text{supp}(\rho)$ as the support of distribution $\rho$.

2. Problem and Method

We focus on two-layer networks for analysis. Assume we are given a pre-trained large neural network consisting of $N$ neurons,

$$f_{[N]}(x) = \sum_{i=1}^{N} \sigma(x; \theta_i)/N,$$

where $\sigma(x; \theta_i)$ denotes the $i$-th neuron with parameter $\theta_i \in \mathbb{R}^d$ and input $x$. In this work, we consider

$$\sigma(x; \theta_i) = b_i \sigma_+(a_i^\top x),$$

where $\theta_i = [a_i, b_i]$ and $\sigma_+(\cdot)$ is an activation function such as Tanh and ReLU. But our algorithm works for general forms of $\sigma(x; \theta_i)$. Given an observed dataset $D_m := (x^{(i)}, y^{(i)})_{i=1}^m$ with $m$ data points, we consider the following regression loss of network $f$:

$$\mathcal{L}[f] = \mathbb{E}_{(x,y) \sim D_m} [(f(x) - y)^2]/2.$$
We are interested in finding a subset $S$ of $n$ neurons ($n < N$) from the large network, which minimizes the loss of the subnetwork $f_S(x) = \sum_{i \in S} \sigma(x; \theta_i) / |S|$, i.e.,

$$\min_{S \subseteq [N]} L[f_S] \quad \text{s.t.} \quad |S| \leq n.$$  

(1)

This is a challenging combinatorial optimization problem. We propose a greedy forward selection strategy, which starts from an empty network and gradually adds the neuron that yields the best immediate decrease on loss. Specifically, starting from $S_0 = \emptyset$, we sequentially add neurons via

$$S_{n+1} \leftarrow S_n \cup \alpha_n^* \quad \text{where} \quad \alpha_n^* = \arg \min_{i \in [N]} L[f_{S_n \cup \{i\}}].$$  

(2)

Notice that the constructed subnetwork inherits the weights of the large network and in practice we may further finetune the subnetwork with training data. More details of the practical algorithm and its extension to deep neural networks are in Section 4.

3. Theoretical Analysis

The simple greedy procedure yields strong theoretical guarantees, which, as a byproduct, also implies the existence of small and accurate subnetworks. Our results are two fold:

i) Under mild conditions, the selected subnetwork of size $n$ achieves $L[f_{S_n}] = \mathcal{O}(1/n) + L_N^\ast$, where $L_N^\ast$ is the best possible loss achievable by convex combinations of all the $N$ neurons in $f_{[N]}$.

ii) We achieve a faster rate of $L[f_{S_n}] = \mathcal{O}(1/n^2)$ if the large network $f_{[N]}$ is sufficiently over-parameterized and can overfit the training data subject to small perturbation (see Assumption 2).

In comparison, the mean field analysis of Song et al. (2018); Mei et al. (2019) shows that:

iii) Training a network of size $n$ using (continuous time) gradient descent starting from random initialization gives an $\mathcal{O}(1/n + \varepsilon)$ loss, where $\varepsilon$ is a (typically small) term involving the loss of infinitely wide networks trained with gradient dynamics. See Song et al. (2018); Mei et al. (2019) for details.

Our fast $\mathcal{O}(1/n^2)$ rate shows that subnetwork selection from large, over-parameterized models yields provably better results than training small networks of the same size starting from scratch using gradient descent. This provides the first theoretical justification of the empirical successes of the popular network pruning paradigm.

We now introduce the theory in depth. We start with the general $\mathcal{O}(1/n)$ rate in Section 3.1, and then establish and discuss the faster $\mathcal{O}(1/n^2)$ rate in Section 3.2 and 3.3.

3.1. General Convergence Rate

Let $L_N^\ast$ be the minimal loss achieved by the best convex combination of all the $N$ neurons in $f_{[N]}$, that is,

$$L_N^\ast = \min_{\alpha = [\alpha_1, \ldots, \alpha_N]} \left\{ L[f_\alpha] : \alpha_i \geq 0, \sum_{i=1}^N \alpha_i = 1 \right\},$$  

(3)

where $f_\alpha = \sum_{i=1}^N \alpha_i \sigma(\theta_i, x)$. It is obvious that $L_N^\ast \leq L[f_{[N]}]$. We can establish the general $\mathcal{O}(1/n)$ rate with the following mild regularity conditions.

**Assumption 1 (Boundedness and Smoothness).** Suppose that $\|\mathbf{x}^{(i)}\| \leq c_1$, $\|y^{(i)}\| \leq c_1$ for every $i \in [m]$, and $\|\sigma_+\|_{Lip} \leq c_1$, $\|\sigma_\ast\|_\infty \leq c_1$ for some $c_1 < \infty$.

**Proposition 1.** Under Assumption 1, if $S_n$ is constructed by (2), we have $L[f_{S_n}] = \mathcal{O}(1/n) + L_N^\ast$, for $\forall n \in [N]$.

Note that the condition of Proposition 1 is very mild. It holds for any original network $f_{[N]}$ of any size, although it is favorable to make $N$ large to obtain a small $L_N^\ast$. In the sequel, we show that a faster $\mathcal{O}(1/n^2)$ rate can be achieved, if $f_{[N]}$ is sufficiently large and can “overfit” the training data in a proper sense.

3.2. Faster Rate With Over-parameterized Networks

We now establish the faster rate $L[f_{S_n}] = \mathcal{O}(1/n^2)$ when the large network is properly over-parametrized, which outperforms the $\mathcal{O}(1/n)$ rate achieved by standard gradient descent. This provides a theoretical foundation for the widely used approach of learning small networks by pruning from large networks.

Specifically, our result requires that $N$ is sufficiently large and the neurons in $f_{[N]}$ are independent and diverse enough such that we can use a convex combination of $N$ neurons to perfectly fit the data $D_m$, even when subject to arbitrary perturbations on the labels with bounded magnitude.

**Assumption 2 (Over-parameterization).** There exists a constant $\gamma > 0$ such that for any $\mathbf{e} = [\mathbf{e}^{(1)}, \ldots, \mathbf{e}^{(m)}] \in \mathbb{R}^m$ with $\|\mathbf{e}\| \leq \gamma$, there exists $[\alpha_1, \ldots, \alpha_N] \in \mathbb{R}^N$ (which may depend on $\mathbf{e}$) with $\alpha_i \in [0, 1]$ and $\sum_{i=1}^N \alpha_i = 1$ such that for all $(\mathbf{x}^{(i)}, y^{(i)})$, $i \in [m],$

$$\sum_{j=1}^N \alpha_j \sigma(\theta_{i,j}, \mathbf{x}^{(i)}) = y^{(i)} + \mathbf{e}^{(i)}.$$  

Note that this implies that $L_N^\ast = 0$.

This roughly requires that the original large network should be sufficiently over-parametrized to have more independent neurons than data points to overfit arbitrarily perturbed labels (with a bounded magnitude). As we discuss in Appendix 9, Assumption 2 can be shown to be equivalent to the interior point condition of Frank-Wolfe algorithm (Bach et al., 2012; Lacoste-Julien, 2016; Chen et al., 2012).
Theorem 2 (Faster Rate). Under assumption 1 and 2, for $S_n$ defined in (2), we have
\[
\mathcal{L}[f_{S_n}] = O(1/(\min(1, \gamma)n)^2).
\] (4)

3.3. Assumption 2 Under Gradient Descent

In this subsection, we show that Assumption 2 holds with high probability when $N$ is sufficiently large and the large network $f_{[N]}$ is trained using gradient descent with a proper random initialization. Our analysis builds on the mean field analysis of neural networks (Song et al., 2018; Mei et al., 2019). We introduce the background before we proceed.

Gradient Dynamics Assume the parameters $\{\theta_i\}_{i=1}^N$ of $f_{[N]}$ are trained using a continuous-time gradient descent (which can be viewed as gradient descent with infinitesimal step size), with a random initialization:
\[
\frac{d}{dt}\theta_i(t) = g_i(\theta(t)), \quad \theta_i(0) \overset{i.i.d.}{=} \rho_0, \quad \forall i \in [N],
\] (5)
where $g_i(\theta)$ denotes the negative gradient of loss w.r.t. $\theta_i$, $g_i(\theta(t)) = \mathbb{E}_{(x,y) \sim D_m}[(y - f(x; \theta(t)))\nabla_\theta \sigma(x, \theta_i(t))]$, and $f(x; \theta) = \sum_{i=1}^N \sigma(x, \theta_i)/N$. Here we initialize $\theta_i(0)$ by drawing i.i.d. samples from some distribution $\rho_0$.

Assumption 3. Assume $\rho_0$ is an absolute continuous distribution on $\mathbb{R}^d$ with a bounded support. Assume the parameters $\{\theta_i\}_{i=1}^N$ in $f_{[N]}$ are obtained by running (5) for some finite time $T$, that is, $\theta_i = \theta_i(T), \forall i \in [N]$.

Mean Field Limit We can represent a neural network using the empirical distribution of the parameters. Let $\rho_t^N$ be the empirical measure of $\{\theta_i(t)\}_{i=1}^N$ at time $t$, i.e., $\rho_t^N := \sum_{i=1}^N \delta_{\theta_i(t)}/N$ where $\delta_{\theta}$ is Dirac measure at $\theta$. We can represent the network $f(x; \theta(t))$ by $f_{\rho_t^N} := \mathbb{E}_{\theta \sim \rho_t^N}[\sigma(x, \theta)]$. Also, $f_{[N]} = f_{\rho_T^N}$ under Assumption 3.

The mean field analysis amounts to study the limit behavior of the neural network with an infinite number of neurons. Specifically, as $N \to \infty$, it can be shown that $\rho_t^N$ weakly converges to a limit distribution $\rho_\infty$, and $f_{\rho_\infty}$ can be viewed as the network with infinite number of neurons at training time $t$. It is shown that $\rho_\infty$ is characterized by a partial differential equation (PDE) (Song et al., 2018; Mei et al., 2019):
\[
\frac{d}{dt} \rho_\infty = \nabla \cdot (\rho_\infty g[\rho_\infty]), \quad \rho_0 = \rho_0,
\] (6)
where $g[\rho_\infty](\theta) = \mathbb{E}_{(x,y) \sim D_m}[(y - f_{\rho_\infty}(x))\nabla_\theta \sigma(x, \theta)]$, $f_{\rho_\infty}(x) = \mathbb{E}_{\theta \sim \rho_\infty}[\sigma(x, \theta)]$, and $\nabla \cdot g$ is the divergence operator.

The mean field theory needs the following smoothness condition on activation to make sure the PDE (6) is well defined (Song et al., 2018; Mei et al., 2019).

Assumption 4. The derivative of activation function is Lipschitz continuous, i.e., $|\sigma'|_{Lip} < \infty$.

It is noticeable that Assumption 4 does not hold for ReLU. However, as shown in Song et al. (2018), empirically, ReLU networks behave very similarly to networks with smooth activation.

A key result of the mean field theory says that $\rho_T^N$ weakly converges to $\rho_\infty$ when $N \to \infty$. It implies that $\mathcal{L}[f_{\rho_\infty}] = O(1/n + \epsilon)$, with $\epsilon = O[\mathcal{L}[f_{\rho_T^N}]]$. As shown in Song et al. (2018), $\mathcal{L}[f_{\rho_T^N}]$ is usually a small term giving that the training time $T$ is sufficiently large, under some regularity conditions.

Over-parameterization of Mean Field Limit The key idea of our analysis is: if the infinitely wide limit network $f_{\rho_T^N}$ can overfit any noise with bounded magnitude (as defined in Assumption 2), then Assumption 2 holds for $f_{\rho_T^N}$ with high probability when $N$ is sufficiently large.

Assumption 5. There exists $\gamma^* > 0$, such that for any noise vector $\epsilon = [\epsilon_i]_{i=1}^n$ with $\|\epsilon\| \leq \gamma^*$, there exists a positive integer $M$, and $[\alpha_1, ..., \alpha_M] \in \mathbb{M}$ with $\alpha_j \in [0, 1]$ and $\sum_{j=1}^M \alpha_j = 1$ and $\theta_j \in supp(\rho_T^N), j \in [M]$ such that
\[
\sum_{j=1}^M \alpha_j \sigma(\theta_j, x^{(i)}) = y^{(i)} + \epsilon^{(i)},
\]
holds for any $i \in [n]$. Here $M, \{\alpha_j, \theta_j\}$ may depend on $\epsilon$.

Assumption 5 can be viewed as an infinite variant of Assumption 2. It is very mild because $supp(\rho_T^N)$ contains infinitely many neurons and given any $\epsilon$, we can pick an arbitrarily large number of neurons from $supp(\rho_T^N)$ and reweight them to fit the perturbed data. Also, assumption 5 implicitly requires a sufficient training time $T$ in order to make the limit network fit the data well.

Assumption 6 (Density Regularity). For $\forall r_0 \in (0, \gamma^*], \exists r_0$ that depends on $r_0$, such that for every $\theta \in supp(\rho_T^N)$, we have $\mathbb{P}_{\theta \sim \rho_T^N}(\|\theta - \bar{\theta}\| \leq r_0) \geq p_0$.

Theorem 3. Suppose Assumption 1, 3, 4, 5 and 6 hold, then for any $\delta > 0$, when $N$ is sufficiently large, assumption 2 holds for any $\gamma \leq \frac{1}{2}\gamma^*$ with probability at least $1 - \delta$, which gives that $\mathcal{L}[f_S] = O(1/(\min(1, \gamma)n)^2)$.

Theorem 3 shows that if the pre-trained network is sufficiently large, the loss of the pruned network decays at a faster rate. Compared with Proposition 1, it highlights the importance of using a large pre-trained network for pruning.

Pruning vs. GD: Numerical Verification of the Rates We numerically verify the fast $O(1/n^2)$ rate in (4) and the $O(1/n)$ rate of gradient descent by Song et al. (2018); Mei
et al. (2019) (when \( \varepsilon \) term is very small). Given some simulated data, we first train a large network \( f_{[N]} \) with \( N = 1000 \) neurons by gradient descent with random initialization. We then apply our greedy selection algorithm to find subnetworks with different sizes \( n \). We also directly train networks of size \( n \) with gradient descent. See Appendix 7 for more details. Figure 2 plots the the loss \( \mathcal{L}[f] \) and the number of neurons \( n \) of the pruned network and the network from scratch. This empirical result matches our \( O(1/n^2) \) rate in Theorem 3, and the \( O(1/n) \) rate of the gradient descent.

3.4. Further Discussion

To the best of our knowledge, our work provides the first rigorous theoretical justification that pruning from over-parameterized models outperforms direct training of small networks from scratch using gradient descent, under rather practical assumptions. However, there still remain gaps between theory and practice that deserves further investigation in future works. Firstly, we only analyze the simple two-layer networks but we believe our theory can be generalized to deep networks with refined analysis and more complex theoretical framework such as deep mean field theory (Araújo et al., 2019; Nguyen & Pham, 2020). We conjecture that pruning deep network gives \( O(1/n^2) \) rate with the constant depending on the Lipschitz constant of the mapping from feature map to output. Secondly, as we only analyze the two-layer networks, our theory cannot characterize whether pruning finds good structure of deep networks, as discussed in Liu et al. (2019b). Indeed, theoretical works on how network architecture influences the performance are still largely missing. Finally, some of our analysis is built on the mean field theory, which is a special parameterization of network. It is also of interest to generalize our theory to other parameterizations.

Algorithm 1 Layer-wise Greedy Subnetwork Selection

**Goal:** Given a pretrained network \( f_{\text{Large}} \) with \( H \) layers, find a subnetwork \( f \) with high accuracy.

Set \( f = f_{\text{Large}} \).

for Layer \( h \in [H]\) (From input layer to output layer) do
  Set \( S = \emptyset \).
  while Convergence criterion is not met do
    Randomly sample a mini-batch data \( \mathcal{D} \).
    for filter (or neuron) \( k \in [N_h] \) do
      \[ S'_k \leftarrow S \cup \{ k \} \]
      Replace layer \( h \) of \( f \) by \( \sum_{j \in [S'_h]} \sigma(\theta_j, z^m) / |S'_h| \)
      Calculate its loss \( \ell_k \) on mini-batch data \( \mathcal{D} \).
    end for
    \[ S \leftarrow S \cup \{ k^* \}, \quad k^* = \arg \min_{k \in [N_h]} \ell_k \]
  end while

Replace layer \( h \) of \( f \) by \( \sum_{j \in [S]} \sigma(\theta_j, z^m) / |S| \).

end for

Finetune the subnetwork \( f \).

4. Practical Algorithm and Experiments

Practical Algorithm We propose to apply the greedy selection strategy in a layer-wise fashion in order to prune neural networks with multiple layers. Assume we have a pretrained deep neural network with \( H \) layers, whose \( h \)-th layer contains \( N_h \) neurons and defines a mapping \( \sum_{j \in [N_h]} \sigma(\theta_j, z^m) / N_h \), where \( z^m \) denotes the input of this layer. To extend the greedy subnetwork selection to deep networks, we propose to prune the layers sequentially, from the input layer to the output layer. For each layer, we first remove all the neurons in that layer, and gradually add the best neuron back that yields the largest decrease of the loss, similar to the updates in (2). After finding the subnetwork for all the layers, we further finetune the pruned network, training it with stochastic gradient descent using the weight of original network as initialization. This allows us to inherit the accuracy and information in the pruned subnetwork, because finetuning can only decrease the loss over the initialization. We summarize the detailed procedure of our method in Algorithm 1.

Empirical Results We first apply the proposed algorithm to prune various models, e.g. ResNet (He et al., 2016), MobileNetV2 (Sandler et al., 2018), MobileNetV3 (Howard et al., 2019) and ProxylessNet (Cai et al., 2019) for ImageNet (Deng et al., 2009) classification. We also show the experimental results on CIFAR-10/100 in the appendix. Our results are summarized as follows:

i) Our greedy selection method consistently outperforms the prior arts on network pruning on learning small and accurate networks with high computational efficiency.
| Model          | Method                        | Top-1 Acc | Size (M) | FLOPS  |
|---------------|-------------------------------|-----------|----------|--------|
|               | Full Model (He et al., 2016)  | 73.4      | 21.8     | 3.68G  |
| ResNet34      | Li et al. (2017)              | 72.1      | -        | 2.79G  |
|               | Liu et al. (2019b)            | 72.9      | -        | 2.79G  |
|               | Dong et al. (2017)            | 73.0      | -        | 2.75G  |
|               | Ours                          | 73.5      | 17.2     | 2.64G  |
| SFP (He et al., 2018a) |                       | 71.8      | -        | 2.17G  |
| FPGM (He et al., 2019) |                      | 72.5      | -        | 2.16G  |
| Ours          |                               | 72.9      | 14.7     | 2.07G  |
| MobileNetV2   | Full Model (Sandler et al., 2018) | 72.0      | 3.5      | 320M   |
|               | Ours                          | 71.9      | 3.2      | 245M   |
|               | LeGR (Chin et al., 2019)      | 71.4      | -        | 224M   |
|               | Uniform (Sandler et al., 2018) | 70.4      | 2.9      | 220M   |
|               | AMC (He et al., 2018b)        | 70.8      | 2.9      | 220M   |
|               | Ours                          | 71.6      | 2.9      | 219M   |
|               | Meta Pruning (Liu et al., 2019a) | 71.2      | -        | 217M   |
|               | Ours                          | 71.2      | 2.7      | 200M   |
| MobileNetV3-Small | Full Model (Howard et al., 2019) | 67.5      | 2.5      | 64M    |
|                | Uniform (Howard et al., 2019) | 65.4      | 2.0      | 47M    |
|                | Ours                          | 65.8      | 2.0      | 49M    |
| ProxylessNet-Mobile | Full Model (Cai et al., 2019) | 74.6      | 4.1      | 324M   |
|                | Uniform (Cai et al., 2019)    | 72.9      | 3.6      | 240M   |
|                | Ours                          | 74.0      | 3.4      | 232M   |

Table 1. Top1 accuracies for different benchmark models, e.g. ResNets (He et al., 2016), MobileNetV2 (Sandler et al., 2018), MobileNetV3-small (Howard et al., 2019) and ProxylessNet (Cai et al., 2019) on ImageNet2012 (Deng et al., 2009).

ii) Finetuning pruned subnetworks of neural architectures (e.g., MobileNetV2/V3) consistently outperforms retraining them from new random initialization, violating the results of Liu et al. (2019b).

iii) Increasing the size of the pre-trained large networks improves the performance of the pruned subnetworks, highlighting the importance of pruning from large models.

4.1. Finding Subnetworks on ImageNet

We use ILSVRC2012, a subset of ImageNet (Deng et al., 2009) which consists of about 1.28 million training images and 50,000 validation images with 1,000 different classes.

Training Details We evaluate each neuron using a minibatch of training data to select the next one to add, as shown in Algorithm 1. We stop adding new neurons when the gap between the current loss and the loss of the original pretrained model is smaller than $\epsilon$. We vary $\epsilon$ to get pruned models with different sizes.

During finetuning, we use the standard SGD optimizer with Nesterov momentum 0.9 and weight decay $5 \times 10^{-5}$. For ResNet, we use a fixed learning rate $2.5 \times 10^{-4}$. For the other architectures, following the original settings (Cai et al., 2019; Sandler et al., 2018), we decay learning rate using cosine schedule (Loshchilov & Hutter, 2017) starting from 0.01. We finetune subnetwork for 150 epochs with batch size 512 on 4 GPUs. We resize images to $224 \times 224$ resolution and adopt the standard data augmentation scheme (mirroring and shifting).
Results Table 1 reports the top1 accuracy, FLOPs and model size \(^1\) of subnetworks pruned from the full networks. We first test our algorithm on two standard benchmark models, ResNet-34 and MobileNetV2. We further apply our algorithm to several recent proposed models e.g., ProxylessNet, MobileNetV3-Small.

ResNet-34 Our algorithm outperforms all the prior results on ResNet-34. We obtain an even better top1 accuracy (73.4% vs. 73.5%) than the full-size network while reducing the FLOPs from 3.68G to 2.64G. We also obtain a model with 72.9% top1 accuracy and 2.07G FLOPs, which has higher accuracy but lower FLOPs than previous works.

MobileNetV2 Different from ResNet and other standard structures, MobileNetV2 on ImageNet is known to be hard to prune using most traditional pruning algorithms (Chin et al., 2019). As shown in Table 1, compared with the ‘uniform baseline’, which uniformly reduces the number of channels on each layer, most popular algorithms fail to improve the performance by a large margin. In comparison, our algorithm improves the performance of small-size networks by a significant margin. As shown in Table 1, the subnetwork with 245M FLOPs achieves 71.9% top1 accuracy, which matches closely with the 72.0% accuracy of the full-size network. Our subnetwork with 151M FLOPs achieves 69.7% top1 accuracy, improving the previous state-of-the-art of 69.4% top1 accuracy with 160M FLOPs. As shown in Figure 3, our algorithm consistently outperforms all the other baselines under all FLOPs. The improvement of our method on the low FLOPs region is particularly significant. For example, when limited to 106M FLOPs, we improve the 65.0% top1 accuracy of Meta Pruning to 66.9%.

ProxlessNet-Mobile and MobileNetV3-Small We further experiment on two recently-proposed architectures, ProxlessNet-Mobile and MobileNetV3-Small. As shown in Table 1, we consistently outperform the ‘uniform baseline’. For MobileNetV3-Small, we improve the 65.4% top1 accuracy to 65.8% when the FLOPs is less than 50M FLOPs. For ProxlessNet-Mobile, we enhance the 72.9% top1 accuracy to 74.0% when the FLOPs is under 240M.

4.2. Rethinking the Value of Finetuning

Recently, Liu et al. (2019b) finds that for ResNet, VGG and other standard structures on ImageNet, re-training the weights of the pruned structure from new random initialization can achieve better performance than finetuning. However, we find that this claim does not hold for mobile models, such as MobileNetV2 and MobileNetV3. In our experiments, we use the same setting of Liu et al. (2019b) for re-training from random initialization.

| Models         | FLOPs | Re-training (%) | Finetune (%) |
|----------------|-------|-----------------|--------------|
| MobileNetV2    | 219M  | 70.8            | 71.6         |
| MobileNetV2    | 169M  | 69.0            | 70.4         |
| MobileNetV3    | 49M   | 63.2            | 65.8         |

Table 2. Top1 accuracy on MobileNetV2 and MobileNetV3-small on ImageNet. “Scratch” denotes training the pruned model from scratch. We use the Scratch-B setting in Liu et al. (2019b) for training from scratch.

We compare finetuning and re-training of the pruned MobileNetV2 with 219M and 169M Flops. As shown in Table 2, finetuning outperforms re-training by a large margin. For example, for the 169M FLOPs model, re-training decreases the top1 accuracy from 70.4% to 69.0%. This empirical evidence demonstrates the importance of using the weights learned by the large model to initialize the pruned model.

We conjecture that the difference between our findings and Liu et al. (2019b) might come from several reasons. Firstly, for large architecture such as VGG and ResNet, the pruned model is still large enough (e.g. as shown in Table 1, FLOPs > 2G) to be optimized from scratch. However, this does not hold for the pruned mobile models, which is much smaller. Secondly, Liu et al. (2019b) mainly focus on sparse regularization based pruning methods such as Han et al. (2015); Li et al. (2017); He et al. (2017). In those methods, the loss used for training the large network has an extra strong regularization term, e.g., channel-wise \(L_p\) penalty. However, when re-training the pruned small network, the penalty is excluded. This gives inconsistent loss functions. As a consequence, the weights of the large pre-trained network may not be suitable for finetuning the pruned model. In comparison, our method uses the same loss for training the re-trained large model and the pruned model.
small network, both without regularization term. A more comprehensive understanding of this issue is valuable to the community, which we leave as a future work.

However, we believe that a more comprehensive understanding of finetuning is valuable to the community, which we leave as a future work.

| Large N → Small N | Original FLOPs (M) | Pruned FLOPs (M) | Top1 Accuracy (%) |
|-------------------|-------------------|-----------------|-------------------|
| Small N           | 320               | 220             | 66.2              |
|                   | 220               | 96              | 65.6              |
|                   | 108               | 97              | 64.9              |

Table 3. We apply our algorithm to get three pruned models with similar FLOPs from full-size MobileNetV2, MobileNetV2×0.75 and MobileNetV2×0.5. We compare their top1 accuracy on ImageNet.

4.3. On the Value of Pruning from Large Networks

Our theory suggests it is better to prune from a larger model, as discussed in Section 3. To verify, we apply our method to MobileNetV2 with different sizes, including MobileNetV2 (full size), MobileNetV2×0.75 and MobileNetV2×0.5 (Sandler et al., 2018). We keep the FLOPs of the pruned models almost the same and compare their performance. As shown in Table 3, the pruned models from larger original models give better performance. For example, the 96M FLOPs pruned model from the full-size MobileNetV2 obtains a top1 accuracy of 66.2% while the one pruned from MobileNetV2×0.5 only has 64.9%.

5. Related Works

Structured Pruning A vast literature on structured pruning (e.g., Han et al., 2016a), which prunes neurons, channels or other units of neural networks. Compared with weight pruning (e.g., Han et al., 2016b), which specifies the connectivity of neural networks, structured pruning is more realistic as it can compress neural networks without dedicated hardware or libraries. Existing methods prune the redundant neurons based on different criterion, including the norm of the weights (e.g., Liu et al., 2017; Zhuang et al., 2018; Li et al., 2017), feature reconstruction error of the next or final layers (e.g., He et al., 2017; Yu et al., 2018; Luo et al., 2017), or gradient-based sensitivity measures (e.g., Baykal et al., 2019b; Zhuang et al., 2018). Our method is designed to directly minimize the final loss, and yields both better practical performance and theoretical guarantees.

Forward Selection vs. Backward Elimination Many of the popular conventional network pruning methods are based on backward elimination of redundant neurons (e.g. Liu et al., 2017; Li et al., 2017; Yu et al., 2018), and fewer algorithms are based forward selection like our method (e.g. Zhu et al., 2018). Among the few exceptions, Zhu et al. (2018) propose a greedy channel selection algorithm similar to ours, but their method is based on minimizing a gradient-norm based sensitivity measure (instead of the actual loss like us), and yield no theoretical guarantees.

Sampling-based Pruning Recently, a number of works (Baykal et al., 2019a; Liebenwein et al., 2019; Baykal et al., 2019b; Mussay et al., 2020), proposed to procedures for pruning networks based on variants of (iterative) random sampling according to certain sensitivity score. These methods can provide concentration bounds on the difference of output between the pruned networks and the full networks, which may yield a bound of $O(1/n + \mathcal{L}[f_{\mathcal{N}}])$ with a simple derivation. Our method uses a simpler greedy deterministic selection strategy and achieves better rate than random sampling in the overparameterized cases. In contrast, sampling-based pruning may not yield the fast $O(1/n^2)$ rate even with overparameterized models. Unlike our method, these works do not justify the advantage of pruning from large models over direct gradient training.

Lottery Ticket; Re-train After Pruning Frankle & Carbin (2019) proposed the Lottery Ticket Hypothesis, claiming the existence of winning subnetworks inside large models. Liu et al. (2019b) regards pruning as a kind for neural architecture search. A key difference between our work and Frankle & Carbin (2019) and Liu et al. (2019b) is how the parameters of the subnetwork are trained:

i) We finetune the parameters of the subnetworks starting from the weights of the pre-trained large model, hence inheriting the information the large model.

ii) Liu et al. (2019b) proposes to re-train the parameters of the pruned subnetwork starting from new random initialization.

iii) Frankle & Carbin (2019) proposes to re-train the pruned subnetwork starting from the same initialization and random seed used to train the pre-trained model.

Obviously, the different parameter training of subnetworks should be combined with different network pruning strategies to achieve the best results. Our algorithmic and theoretical framework naturally justifies the finetuning approach. Different theoretical frameworks for justifying the proposals of Liu et al. (2019b) and Frankle & Carbin (2019) (equipped with their corresponding subnetwork selection methods) are of great interest.

More recently, a concurrent work Malach et al. (2020) discussed a stronger form of lottery ticket hypothesis that shows the existence of winning subnetworks in large net-
works with random weights (without pre-training), which corroborates the empirical observations in (Wang et al., 2019; Ramanujan et al., 2019). However, the result of Malach et al. (2020) does not yield fast rate as our framework for justifying the advantage of network pruning over training from scratch, and does not motivate practical algorithms for finding good subnetworks in practice.

Frank-Wolfe As suggested in Bach (2017), Frank-Wolfe (Frank & Wolfe, 1956) can be applied to learn neural networks, which yields an algorithm that greedily adds neurons to progressively construct a network. However, each step of Frank-Wolfe leads to a challenging global optimization problem, which can not be solved in practice.

Compared with Bach (2017), our subnetwork selection approach can be viewed as constraining the global optimization the discretized search space constructed using over-parameterized large networks pre-trained using gradient descent. Because gradient descent on over-parameterized networks is shown to be nearly optimal (e.g., Song et al., 2018; Mei et al., 2019; Du et al., 2018; 2019; Jacot et al., 2018), selecting neurons inside the pre-trained models can provide a good approximation to the original non-convex problem.

Sub-modular Optimization An alternative general framework for analyzing greedy selection algorithms is based on sub-modular optimization (Nemhauser et al., 1978). However, our problem is not sub-modular, and the (weak) sub-modular analysis (Das & Kempe, 2011) can only bound the ratio between $L[f_S]$ and the best loss of subnetworks of size $n$ achieved by (1), not the best loss $L^*_N$ achieved by the best convex combination of all the $N$ neurons in the large model.

6. Conclusion

We propose a simple and efficient greedy selection algorithm for constructing subnetworks from pretrained large networks. Our theory provably justifies the advantage of pruning from large models over training small networks from scratch. The importance of using sufficiently large, over-parameterized models and finetuning (instead of retraining) the selected subnetworks are emphasized. Empirically, our experiments verify our theory and show that our method improves the prior arts on pruning various models such as ResNet-34 and MobileNetV2 on Imagenet.

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7. Details for the Toy Example

Suppose we train the network with \( n \) neurons for \( T \) time using gradient descent with random initialization, i.e., the network we obtain is \( f_{\rho_T} \), using the terminology in Section 3.3. As shown by Song et al. (2018); Mei et al. (2019), \( \mathcal{L}[f_{\rho_T}] \) is actually \( O(1/n + \epsilon) \) with high probability, where \( \epsilon = \mathcal{L}[f_{\rho_T^\infty}] \) is the loss of the mean field limit network at training time \( T \). Song et al. (2018) shows that \( \lim_{T \to \infty} \mathcal{L}[f_{\rho_T^\infty}] = 0 \) under some regularity conditions and this implies that if the training time \( T \) is sufficient, \( \mathcal{L}[f_{\rho_T^\infty}] \) is generally a smaller term compared with the \( O(1/n) \) term.

To generate the synthesis data, we first generate a neural network \( f_{\text{gen}}(x) = \frac{1}{1000} \sum_{i=1}^{N} b_i \sigma(a_i^T x) \), where \( a_i \) are i.i.d. sample from a 10 dimensional standard Gaussian distribution and \( b_i \) are i.i.d. sample from a uniform distribution \( \text{Unif}(-5,5) \). The training data \( x \) is also generated from a 10 dimensional standard Gaussian distribution. We choose \( f_{\text{gen}}(x) = y \) as the label of data. Our training data consists of 100 data points. The network we use to fit the data is \( f = \frac{1}{n} \sum_{i=1}^{n} b_i \tanh(a_i^T x) \). We use network with 1000 neurons for pruning and the pruned models will not be finetuned. All networks are trained for same and sufficiently large time to converge.

8. Finding Sub-Networks on CIFAR-10/100

In this subsection, we display the results of applying our proposed algorithm to various model structures on CIFAR-10 and CIFAR-100. On CIFAR-10 and CIFAR-100, we apply our algorithm to the networks already pruned by network slimming (Liu et al., 2017) provided by Liu et al. (2019b) and show that we can further compress models which have already pruned by the \( L_1 \) regularization. We apply our algorithm on the pretrained models, and finetune the model with the same experimental setting as ImageNet.

As demonstrated in Table 4, our proposed algorithm can further compress a model pruned by Liu et al. (2019b) without or only with little drop on accuracy. For example, on the pretrained VGG19 on CIFAR-10, Liu et al. (2017) can prune 30% channels and get 93.81\% \pm 0.14\% accuracy. Our algorithm can prune 44% channels of the original VGG19 and get 93.78\% \pm 0.16\% accuracy, which is almost the same as the strong baseline number reported by Liu et al. (2019b).

| Dataset   | Model       | Method         | Prune Ratio (%) | Accuracy (%) |
|-----------|-------------|----------------|-----------------|--------------|
| CIFAR10   | VGG19       | Liu et al. (2017) | 70           | 93.81 \pm 0.14 |
|           |             | Ours           | 56           | 93.78 \pm 0.16 |
|           | PreResNet-164 | Liu et al. (2017) | 60           | 94.90 \pm 0.04 |
|           |             | Ours           | 51           | 94.91 \pm 0.06 |
|           |             | Liu et al. (2017) | 40           | 94.71 \pm 0.21 |
|           |             | Ours           | 33           | 94.68 \pm 0.17 |
| CIFAR100  | VGG19       | Liu et al. (2017) | 50           | 73.08 \pm 0.22 |
|           |             | Ours           | 44           | 73.05 \pm 0.19 |
|           | PreResNet-164 | Liu et al. (2017) | 60           | 76.68 \pm 0.35 |
|           |             | Ours           | 53           | 76.63 \pm 0.37 |
|           |             | Liu et al. (2017) | 40           | 75.73 \pm 0.29 |
|           |             | Ours           | 37           | 75.74 \pm 0.32 |

Table 4. Accuracy on CIFAR100 and CIFAR10. “Prune ratio” stands for the total percentage of channels that are pruned in the whole network. We apply our algorithm on the models pruned by Liu et al. (2017) and find that our algorithm can further prune the models. The performance of Liu et al. (2017) is reported by Liu et al. (2019b). Our reported numbers are averaged by five runs.

9. Discussion on Assumption 2 and 5

Let \( \phi_i(\theta) = \sigma(x^{(j)}; \theta) / \sqrt{m} \) and \( \phi(\theta) = [\phi_1(\theta), \ldots, \phi_m(\theta)] \) to be the vector of the outputs of the neuron \( \sigma(x; \theta) \) scaled by \( 1/\sqrt{m} \), realized on a dataset \( D_m := \{x^{(j)}\}^m_{j=1} \). We call \( \phi(\theta) \) the feature map of \( \theta \). Given a large network \( f_{|N|}(x) = \sum_{i=1}^{N} \sigma(x; \theta_i) / N \), define the marginal polytope of the feature map to be

\[
\mathcal{M}_N := \text{conv} \{ \phi(\theta_i) \mid i \in \{1, \ldots, N\} \},
\]

where \( \text{conv} \) denotes the convex hull. Then it is easy to see that Assumption 2 is equivalent to saying that \( y := [y^{(1)}, \ldots, y^{(m)}] / \sqrt{m} \) is in the interior of the marginal polytope \( \mathcal{M}_N \), i.e., there exists \( \gamma > 0 \) such that \( B(y, \gamma) \subseteq \mathcal{M}_N \).
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Here we denote by $B(\mu, r)$ the ball with radius $r$ centered at $\mu$. Similar to Assumption 2, Assumption 5 is equivalent to require that $B(y, \gamma^*) \subseteq M$, where

$$M := \text{conv} \{ \phi(\theta) \mid \theta \in \text{supp}(\rho_N^T) \}.$$ 

We may further relax the assumption to assuming $y$ is in the relative interior (instead of interior) of $M_N$ and $M$. However, this requires some refined analysis and we leave this as future work.

It is worth mention that when $M$ has dimension $m$ and $f_{\rho_N^T}$ gives zero training loss, then assumption 5 holds. Similarly, if $M_N$ has dimension $m$ and $f_{\rho_N^T}$ gives zero training loss, then assumption 2 holds.

10. Proofs

Our proofs use the definition of the convex hulls defined in Section 9 of Appendix.

10.1. Proof of Proposition 1

The proof of Proposition 1 follows the standard argument of proving the convergence rate of Frank-Wolfe algorithm with some additional arguments. Our algorithm is not a Frank-Wolfe algorithm, but as illustrated in the subsequent proof, we can essentially use the Frank-Wolfe updates to control the error of our algorithm.

Define $\ell(u) = \|u - y\|^2$, then the subnetwork selection problem can be viewed as solving

$$\min_{u \in \mathcal{M}_N} \ell(u),$$

with $\mathcal{L}^* = \min_{u \in \mathcal{M}_N} \ell(u)$. And our algorithm can be viewed as starting from $u^0 = 0$ and iteratively updating $u$ by

$$u^k = (1 - \xi_k)u^{k-1} + \xi_k q^k, \quad q^k = \arg\min_{q \in \text{Vert}(\mathcal{M}_N)} \ell((1 - \xi_k)u^{k-1} + \xi_k q), \quad (7)$$

where $\text{Vert}(\mathcal{M}_N) := \{ \phi(\theta_1), ..., \phi(\theta_N) \}$ denotes the vertices of $\mathcal{M}_N$, and we shall take $\xi_k = 1/k$. We aim to prove that $\ell(u^k) = O(1/k) + \mathcal{L}^*_N$. Our proof can be easily extended to general convex functions $\ell(\cdot)$ and different $\xi_k$ schemes.

By the convexity and the quadratic form of $\ell(\cdot)$, for any $s$, we have

$$\ell(s) \geq \ell(u^{k-1}) + \nabla \ell(u^{k-1})^T (s - u^{k-1}) \quad (8)$$

$$\ell(s) \leq \ell(u^{k-1}) + \nabla \ell(u^{k-1})^T (s - u^{k-1}) + \|s - u^{k-1}\|^2. \quad (9)$$

Minimizing $s$ in $\mathcal{M}_N$ on both sides of (8), we have

$$\mathcal{L}_N^* = \min_{s \in \mathcal{M}_N} \ell(s) \geq \min_{s \in \mathcal{M}_N} \{ \ell(u^{k-1}) + \nabla \ell(u^{k-1})^T (s - u^{k-1}) \}$$

$$\quad = \ell(u^{k-1}) + \nabla \ell(u^{k-1})^T (s^k - u^{k-1}), \quad (10)$$

Here we define

$$s^k = \arg\min_{s \in \mathcal{M}_N} \nabla \ell(u^{k-1})^T (s - u^{k-1})$$

$$= \arg\min_{s \in \text{Vert}(\mathcal{M}_N)} \nabla \ell(u^{k-1})^T (s - u^{k-1}), \quad (11)$$

where the second equation holds because we optimize a linear objective on a convex polytope $\mathcal{M}_N$ and hence the solution must be achieved on the vertices $\text{Vert}(\mathcal{M}_N)$. Note that if we update $u^k$ by $u^k = (1 - \xi_k)u^{k-1} + \xi_k s^k$, we would get the standard Frank-Wolfe (or conditional gradient) algorithm. The difference between our method and Frank-Wolfe is that we greedily minimize the loss $\ell(u^k)$, while the Frank-Wolfe minimizes the linear approximation in (11).

Define $D_{\mathcal{M}_N} := \max_{u,v} \{\|u - v\| : u, v \in \mathcal{M}_N\}$ to be the diameter of $\mathcal{M}_N$. Following (14), we have

$$\ell(u^k) \leq \ell((1 - \xi_k)u^{k-1} + \xi_k q)$$

$$\leq \ell((1 - \xi_k)u^{k-1} + \xi_k s^k)$$

$$\leq \ell(u^{k-1}) + \xi_k \nabla \ell(u^{k-1})^T (s^k - u^{k-1}) + C\xi_k^2$$

$$\leq (1 - \xi_k)\ell(u^{k-1}) + \xi_k \mathcal{L}_N^* + C\xi_k^2, \quad (12)$$

$$\leq (1 - \xi_k)\ell(u^{k-1}) + \xi_k \mathcal{L}_N^* + C\xi_k^2, \quad (13)$$
where we define \( C := D_{MN}^2 \). (12) follows (9), and (13) follows (10). Rearranging this, we get

\[
\ell(u^k) - \mathcal{L}_N^* - C\xi_k \leq (1 - \xi_k) (\ell(u^{k-1}) - \mathcal{L}_N^* - C\xi_{k})
\]

By iteratively applying the above inequality, we have

\[
\ell(u^k) - \mathcal{L}_N^* - C\xi_k \leq \prod_{i=1}^{k} (1 - \xi_i) (\ell(u^0) - \mathcal{L}_N^* - C\xi_1).
\]

Taking \( \xi_k = 1/k \). We get

\[
\ell(u^k) - \mathcal{L}_N^* - C/k \leq \frac{1}{k} (\ell(u^0) - \mathcal{L}_N^* - C).
\]

And thus

\[
\ell(u^k) \leq \frac{1}{k} (\ell(u^0) - \mathcal{L}_N^*) + \mathcal{L}_N^* = \mathcal{O}\left(\frac{1}{k}\right) + \mathcal{L}_N^*.
\]

This completes the proof.

### 10.2. Proof of Theorem 2

The proof leverages the idea from the proof of Proposition 1 of Chen et al. (2012) for analyzing their Herding algorithm, but contains some extra nontrivial argument.

Following the proof of Proposition 1, our problem can be viewed as

\[
\min_{\mathbf{u} \in \mathcal{M}_N} \left\{ \ell(\mathbf{u}) := \|\mathbf{u} - \mathbf{y}\|^2 \right\},
\]

with \( \mathcal{L}_N^* = \min_{\mathbf{u} \in \mathcal{M}_N} \ell(\mathbf{u}) \), our greedy algorithm can be viewed as starting from \( u^0 = 0 \) and iteratively updating \( u \) by

\[
\mathbf{u}^k = \frac{k - 1}{k} \mathbf{u}^{k-1} + \frac{1}{k} q^k, \quad q^k = \arg \min_{q \in \text{Vert} (\mathcal{M}_N)} \| \frac{k - 1}{k} \mathbf{u}^{k-1} + \frac{1}{k} q - \mathbf{y} \|^2
\]

where \( \text{Vert} (\mathcal{M}_N) := \{ \phi(\theta_1), ..., \phi(\theta_N) \} \) denotes the vertices of \( \mathcal{M}_N \). We aim to prove that \( \ell(u^k) = \mathcal{O}(1/(k \max(1, \gamma))^2) \), under Assumption 2.

Define \( \mathbf{w}^k = k(\mathbf{y} - \mathbf{u}^k) \), then \( \ell(u^k) = \|\mathbf{w}^k\|^2 / k^2 \). Therefore, it is sufficient to prove that \( \|\mathbf{w}^k\| = \mathcal{O}(1/(\max(1, \gamma))) \).

Similar to the proof of Proposition 1, we define

\[
s^{k+1} = \arg \min_{s \in \mathcal{M}_N} \nabla \ell(u^k) \top (s - u^k)
\]

\[
= \arg \min_{s \in \mathcal{M}_N} \nabla \ell(u^k) \top s
\]

\[
= \arg \min_{s \in \mathcal{M}_N} \langle \mathbf{w}^k, s \rangle.
\]

\[
= \arg \min_{s \in \mathcal{M}_N} \langle \mathbf{w}^k, s - \mathbf{y} \rangle.
\]

Because \( B(\mathbf{y}, \gamma) \) is included in \( \mathcal{M}_N \) by Assumption 2, we have \( s' := \mathbf{y} - \gamma \mathbf{w}^k / \|\mathbf{w}^k\| \in \mathcal{M}_N \). Therefore

\[
\langle \mathbf{w}^k, (s^{k+1} - \mathbf{y}) \rangle = \min_{s \in \mathcal{M}_N} \langle \mathbf{w}^k, s - \mathbf{y} \rangle \leq \langle \mathbf{w}^k, (s' - \mathbf{y}) \rangle = -\gamma \|\mathbf{w}^k\|.
\]
Proof.
We prove \( \ell \). This proves that Lemma 5.
Under the Assumption 1, 3, 4, 5 and 6. For any \( u \), we first introduce the following Lemmas.

10.3. Proof of Theorem 3
where \( C \) and \( D \) are two positive numbers. Then we have \( \frac{1}{\min(1, \gamma)} \) for all \( k = 1, 2, \ldots \).

This proves that \( \ell(u^k) = \frac{\|u^k\|^2}{k^2} = \mathcal{O}\left(\frac{1}{k^2 \min(1, \gamma)^2}\right) \).

Lemma 4. Assume \( \{z_k\}_{k \geq 0} \) is a sequence of numbers satisfying \( z_0 = 0 \) and

|\( z_{k+1} \| \leq |z_k|^2 - 2\gamma |z_k| + C, \quad \forall k = 0, 1, 2, \ldots \)

where \( C \) and \( \gamma \) are two positive numbers. Then we have \( |z_k| \leq \max(\sqrt{C}, C/(2\gamma)) \) for all \( k = 0, 1, 2, \ldots \).

Proof. We prove \( |z_k| \leq \max(\sqrt{C}, C/(2\gamma)) := u_* \) by induction on \( k \). Because \( z_0 = 0 \), the result holds for \( k = 0 \). Assume \( |z_k| \leq u_* \), we want to prove that \( |z_{k+1}| \leq u_* \) also holds.

Define \( f(z) = z^2 - 2\gamma z + C \). Note that the maximum of \( f(z) \) on an interval is always achieved on the vertices, because \( f(z) \) is convex.

Case 1: If \( |z_k| \leq C/(2\gamma) \), then we have

|\( z_{k+1} \| \leq f(|z_k|) = \max \left\{ f(z) : z \in [0, C/(2\gamma)] \right\} = \max \left\{ f(0), f(C/(2\gamma)) \right\} = \max \left\{ C, C^2/(4\gamma^2) \right\} \leq u_*^2. \)

Case 2: If \( |z_k| \geq C/(2\gamma) \), then we have

|\( z_{k+1} \| \leq |z_k|^2 - 2\gamma |z_k| + C \leq |z_k|^2 \leq u_*^2. \)

In both cases, we have \( |z_{k+1}| \leq u_* \). This completes the proof. \( \square \)

10.3. Proof of Theorem 3
We first introduce the following Lemmas.

Lemma 5. Under the Assumption 1, 3, 4, 5 and 6. For any \( \delta > 0 \), when \( N \) is sufficient large, with probability at least \( 1 - \delta \),

\[ B \left( y, \frac{1}{2\gamma} \right) \subseteq conv \{ \phi(\theta) : \theta \in supp(\rho_N^\gamma) \}. \]

Here \( \rho_N^\gamma \) is the distribution of the weight of the large network with \( N \) neurons trained by gradient descent.

10.3.1. Proof of Theorem 3
The above lemmas directly imply Theorem 3.
10.3.2. PROOF OF LEMMA 5

In this proof, we simplify the statement that ‘for any $\delta > 0$, when $N$ is sufficiently large, event $E$ holds with probability at least $1 - \delta$’ by ‘when $N$ is sufficiently large, with high probability, event $E$ holds’.

By the Assumption 5, there exists $\gamma^* > 0$ such that

$$B(y, \gamma^*) \subseteq \text{conv}\{\phi(\theta) \mid \theta \in \text{supp}(\rho_N^T)\} = M.$$  

Given any $\theta \in \text{supp}(\rho_N^T)$, (remind that supp denotes support of some distribution) define

$$\phi^N(\theta) = \arg \min_{\theta' \in \text{supp}(\rho_N^T)} \|\phi(\theta') - \phi(\theta)\|$$

where $\phi^N(\theta)$ is the best approximation of $\phi(\theta)$ using the points $\phi(\theta_i), \theta_i \in \text{supp}(\rho_N^T)$.

Using Lemma 9, by choosing $\epsilon = \gamma^*/6$, when $N$ is sufficiently large, we have

$$\sup_{\theta \in \text{supp}(\rho_N^T)} \|\phi(\theta) - \phi^N(\theta)\| \leq \gamma^*/6,$$  

(15) implies that $M_N$ can approximate $M$ for large $N$. Since $M$ is assumed to contain the ball centered at $y$ with radius $\gamma^*$, as $M_N$ approximates $M$, intuitively $M_N$ would also contain the ball centered at $y$ with a smaller radius. And below we give a rigorous proof for this intuition.

**Step 1:** $\|\hat{y} - y\| \leq \gamma^*/6$.  
When $N$ is sufficiently large, with high probability, we have

$$\|\hat{y} - y\| \leq \sum_{i=1}^{M} q_i \|\phi^N(\theta_i^*) - \phi(\theta_i^*)\| \leq \gamma^*/6.$$  

**Step 2** $B(\hat{y}, \frac{2}{3} \gamma^*) \subseteq M$.  
By step one, with high probability, $\|\hat{y} - y\| \leq \gamma^*/6$, which implies that $\hat{y} \in B(y, \gamma^*/6) \subseteq B(y, \gamma^*) \subseteq M$. Also, for any $A \in \partial M$ (here $\partial M$ denotes the boundary of $M$), we have

$$\|\hat{y} - A\| \geq \|y - A\| - \|y - \hat{y}\| \geq \gamma^* - \gamma^*/6.$$  

This gives that $B(\hat{y}, \frac{2}{3} \gamma^*) \subseteq M$.

**Step 3** $B(\hat{y}, \frac{2}{3} \gamma^*) \subseteq M_N$.  
Notice that $\hat{y}$ is a point in $\mathbb{R}^m$ and suppose that $A$ belongs to the boundary of $M_N$ (denoted by $\partial M_N$) such that

$$\|\hat{y} - A\| = \min_{\hat{A} \in \partial M_N} \|\hat{y} - \hat{A}\|.$$  

We prove by contradiction. Suppose that we have $\|\hat{y} - A\| < \frac{2}{3} \gamma^*$.

Using support hyperplane theorem, there exists a hyperplane $P = \{u : \langle u - A, v \rangle = 0\}$ for some nonempty vector $v$, such that $A \in P$ and

$$\sup_{q \in M_N} \langle q, v \rangle \leq \langle A, v \rangle.$$  

We choose $A' \in P$ such that $A' - \hat{y} \perp P$ ($A$ and $A'$ can be the same point). Notice that

$$\|\hat{y} - A'\|^2 = \|\hat{y} - A + A'\|^2 = \|\hat{y} - A\|^2 + \|A - A'\|^2 + 2\langle \hat{y} - A, A - A' \rangle.$$  

Since $A' \perp P$ and $A, A' \in P$, we have $\langle \hat{y} - A, A - A' \rangle = 0$ and thus $\|\hat{y} - A'\| \leq \|\hat{y} - A\| < \frac{2}{3} \gamma^*$. We have

$$A' \in B(\hat{y}, \|\hat{y} - A\|) \subseteq B\left(\hat{y}, \frac{2}{3} \gamma^*\right) \subseteq B\left(\hat{y}, \frac{5}{6} \gamma^*\right) \subseteq M.$$
Notice that as both $\tilde{y}, A' \in \mathcal{M}$ we choose $\lambda \geq 1$ such that $\tilde{y} + \lambda (A' - \tilde{y}) \in \partial \mathcal{M}$, where $\partial \mathcal{M}$ denotes the boundary of $\mathcal{M}$. Define $B = \tilde{y} + \lambda (A' - \tilde{y})$. As we have shown that $B \left( \tilde{y} + \frac{5}{6} \gamma^* \right) \subseteq \mathcal{M}$, we have $\| \tilde{y} - B \| \geq \frac{5}{6} \gamma^*$. And thus

$$\| B - A' \| = \| B - \tilde{y} \| - \| \tilde{y} - A' \|$$

$$> \frac{5}{6} \gamma^* - \frac{2}{3} \gamma^*$$

$$> \frac{1}{6} \gamma^*.$$

Also notice that

$$\langle B - A, v \rangle = \langle \tilde{y} + \lambda (A' - \tilde{y}) - A, v \rangle$$

$$= (1 - \lambda) \langle \tilde{y} - A, v \rangle + \lambda \langle A' - A, v \rangle$$

$$= (1 - \lambda) \langle \tilde{y} - A, v \rangle$$

$$\geq 0.$$

This implies that $B$ and $\mathcal{M}$ are on different side of $P$.

With high probability, we are able to find $D \in \{ \phi(\theta); \theta \in \text{supp}(\rho_N^\gamma) \}$ such that

$$\| D - B \| \leq \gamma^* / 6.$$

By the definition, $D \in \mathcal{M}_N$ and thus $\langle D - A, v \rangle \leq 0$ as shown by the supporting hyperplane theorem. Also remind that $\langle B - A, v \rangle \geq 0$. These allow us to choose $\lambda' \in [0, 1]$ such that

$$\langle \lambda' D + (1 - \lambda') B - A, v \rangle = 0.$$

We define $E = \lambda' D + (1 - \lambda') B$ and thus $E \in P$. Notice that

$$\| B - E \| = \| B - \lambda' D - (1 - \lambda') B \| = \lambda' \| B - D \| \leq \| B - D \| \leq \frac{\gamma^*}{6}.$$

Also,

$$\| B - E \|^2 = \| B - A' + A' - E \|^2 = \| B - A' \|^2 + \| A' - E \|^2 + 2 \langle B - A', A' - E \rangle.$$

As $B - A' \perp P$ and $A', E \in P$, we have $\langle B - A', A' - E \rangle = 0$, which implies that $\| B - E \| \geq \| B - A' \| > \frac{1}{6} \gamma^*$, which makes contradiction.

**Step 4** $B \left( \tilde{y}, \frac{1}{2} \gamma^* \right) \subseteq \mathcal{M}_N$ As for sufficiently large $N$, we have $\| \tilde{y} - y \| \leq \frac{1}{6} \gamma^*$ and thus

$$B \left( \tilde{y}, \frac{1}{2} \gamma^* \right) \subseteq B \left( \tilde{y}, \frac{2}{3} \gamma^* \right) \subseteq \mathcal{M}_N.$$

### 11. Technical Lemmas

**Lemma 6.** Under assumption 1 and 3, for any $N$, at training time $T < \infty$, for any $\theta \in \text{supp}(\rho_N^\gamma)$ or $\theta \in \text{supp}(\rho_\delta^\sigma)$, we have $\| \theta \| \leq C$, $\| \phi(\theta) \| \leq C$ and $\| \phi(\theta) \|_{L^p} \leq C$ for some constant $C < \infty$.

**Lemma 7.** Suppose $\theta_i \in \mathbb{R}^d$, $i = 1, ..., N$ are i.i.d. samples from some distribution $\rho$ and $\Omega \subseteq \mathbb{R}^d$ is bounded. For any radius $r_B > 0$ and $\delta > 0$, define the following two sets

$$A = \{ \theta_B \in \Omega \mid \mathbb{P}_{\theta \sim \rho} (\theta \in B(\theta_B, r_B)) > \frac{4}{N} \left( (d + 1) \log (2N) + \log (8/\delta) \right) \}.$$

$$B = \{ \theta_B \in \Omega \mid \| \theta_B - \theta_B^N \| \leq r_B \},$$

where $\theta_B^N = \arg \min_{\theta' \in \{ \theta_i \}_{i=1}^N} \| \theta_B - \theta' \|$. With probability at least $1 - \delta$, $A \subseteq B$. 

Thus given any $T < \infty$, we have

$$\| \phi(\theta) - \phi(\theta) \| \leq \epsilon,$$

where $\phi(\theta) = \arg \min \| \phi(\theta) - \phi(\theta) \|$ and $\theta_i$ are i.i.d. samples from $\rho_T^\infty$.

**Lemma 9.** For any $\epsilon > 0$ and $\epsilon > 0$, when $N$ is sufficiently large ($N$ depends on $\epsilon$), with probability at least $1 - \epsilon$, we have

$$\sup_{\theta \in \text{supp}(\rho_T^\infty)} \| \phi(\theta) - \phi^N(\theta) \| \leq \epsilon,$$

where $\phi^N(\theta) = \arg \min_{\theta' \in \text{supp}(\rho_T^N)} \| \phi(\theta') - \phi(\theta) \|$.

**11.1. Proof of Lemma 6**

We prove the case of training network with $N$ neurons. Notice that

$$\left\| \frac{\partial}{\partial t} \theta(t) \right\| = \left\| g[\theta(t), \rho_t^N] \right\|$$

$$\leq \sqrt{\mathbb{E}_{x, y \sim D} \left( y - f_{\rho_t^N}(x) \right)^2} \sqrt{\mathbb{E}_{x, y \sim D} \| \nabla_\theta \sigma(\theta(t), x) \|^2}$$

Notice that by the assumption 1, we have $\sqrt{\mathbb{E}_{x, y \sim D} \left( y - f_{\rho_t^N}(x) \right)^2} \leq C$. Remind that $\theta(t) = [\alpha(t), b(t)], \sigma(\theta(t), x) = b(t)\sigma_+(a^T(t)x)$. Thus we have

$$\left\| \frac{\partial}{\partial t} b(t) \right\| \leq C \| \sigma_+ \|_\infty .$$

And thus for any $i \in \{1, \ldots, N\}, \sup_{t \in [0, T]} \| b_i(t) \| \leq \int_0^T \left\| \frac{\partial}{\partial t} b_i(s) \right\| ds \leq TC$. Also

$$\left\| \frac{\partial}{\partial t} \alpha(t) \right\| \leq C \| \alpha \|_\infty \sqrt{\mathbb{E}_{x \sim D} \| x \|^2}$$

$$\leq TC.$$

By assumption 3, that $\| \theta_0(t) \| \leq C$, we have

$$\sup_{t \in [0, T]} \| \theta_1(t) \| \leq \int_0^T \left\| \frac{\partial}{\partial t} \theta_1(s) \right\| ds \leq T^2 C.$$ 

Notice that this also holds to training the network with infinite number of neurons. Notice that $\| \phi(\theta) \| = \sqrt{\frac{1}{m} \sum_{j=1}^m \sigma^2(\theta, x^{(j)})} \leq CT$. And

$$\| \phi(\theta) \|_{\text{Lip}} = \sup_{\theta_1, \theta_2} \frac{\| \phi(\theta_1) - \phi(\theta_2) \|}{\| \theta_1 - \theta_2 \|}$$

$$= \sup_{\theta_1, \theta_2} \sqrt{\frac{1}{m} \sum_{j=1}^m \left( \sigma(\theta_1, x^{(j)}) - \sigma(\theta_2, x^{(j)}) \right)^2} \| \theta_1 - \theta_2 \|$$

$$\leq TC \| \sigma_+ \|_{\text{Lip}} + \| \sigma_+ \|_\infty .$$

Thus given any $T < \infty$, all those three quantities can be bounded by some constant.
11.2. Proof of Lemma 7

The following proof follows line 1 and line 2 of the proof of Lemma 16 of (Chaudhuri & Dasgupta, 2010).

Define $g_{\theta_B}(\theta) = \mathbb{1}\{\theta \in B(\theta_B, r_B)\}$ and $\beta_N = \sqrt{(4/N)(d_{VC} \log 2N + \log(8/\delta))}$, where $d_{VC}$ is the VC dimension of the function class $G = \{g_{\theta_B}, \theta_B \in \Omega\}$ and thus $d_{VC} \leq d + 1$ (Dudley, 1979). Let $E_{g_{\theta_B}} = \mathbb{P}_{\theta \sim \rho}(\theta \in B(\theta_B, r_B))$ and $E_N g_{\theta_B} = \sum_{i=1}^{N} g_{\theta_B}(\theta_i)/N$. So

$$A = \{\theta_B \mid E_{g_{\theta_B}} > \beta_N^2\}$$

and we further define

$$A_2 = \{\theta_B \mid E_N g_{\theta_B} > 0\}.$$

From theorem 15 of (Chaudhuri & Dasgupta, 2010) (which is a rephrase of the generalization bound), we know that: for any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $g_{\theta_B} \in G$,

$$E_{g_{\theta_B}} - E_N g_{\theta_B} \leq \beta_N \sqrt{E_{g_{\theta_B}}}$$

(16)

Notice that for any $g_{\theta_B}$ which satisfies (16),

$$E_{g_{\theta_B}} > \beta_N^2 \Rightarrow E_N g_{\theta_B} > 0$$

So this means: for any $\delta > 0$, with probability at least $1 - \delta$,

$$A \subseteq A_2 = B$$

where the last equality follows from the following:

$$A_2 = \{\theta_B \mid E_N g_{\theta_B} > 0\} = \{\text{there exists some } \theta_i \text{ such that } \theta_i \in B(\theta_B, r_B)\} = B$$

11.3. Proof of Lemma 8

Given $\epsilon > 0$, we choose $r_0$ sufficiently small such that $Cr_0 \leq \epsilon$ (here $C$ is some constant defined in Lemma 6). For this choice of $r_0$, given the corresponding $p_0$ (defined in assumption 6), for any $\delta > 0$, there exists $N(\delta)$ such that $\forall N \geq N(\delta)$, we have

$$p_0 > \frac{4}{N} ((d + 1) \log(2N) + \log(8/\delta)) := \beta_N^2.$$

And thus from assumption 6, we have

$$\forall \theta \in \text{supp}(\rho_T^\infty), \mathbb{P}_{\theta \sim \rho_T} (\theta' \in B(\theta, r_0)) \geq p_0 > \beta_N^2.$$

This implies

$$\text{supp}(\rho_T^\infty) \subseteq A = \{\theta_B \mid \mathbb{P}_{\theta \sim \rho}(\theta \in B(\theta_B, r_0)) > \beta_N^2\}$$

From Lemma 7 (set $r_B = r_0$), we know: with probability at least $1 - \delta$,

$$A \subseteq B = \{\theta_B \in \Omega \mid \|\theta_B - \theta_B^N\| \leq r_0\},$$

Thus, with probability at least $1 - \delta$,

$$\text{supp}(\rho_T^\infty) \subseteq B$$

and this means: with probability at least $1 - \delta$, we have

$$\forall \theta \in \text{supp}(\rho_T^\infty), \|\theta - \theta_B^N\| \leq r_0.$$
Here the last inequality uses Lemma 6.

11.4. Proof of Lemma 9

In this proof, we simplify the statement that ‘for any $\delta > 0$, when $N$ is sufficiently large, event $E$ holds with probability at least $1 - \delta$’ by ‘when $N$ is sufficiently large, with high probability, event $E$ holds’.

Suppose that $\theta_i, i \in [N]$ is the weight of neurons of network $f_{\rho_i}$. Given any $\theta \in \text{supp}(\rho_i)$, define

$$\phi^N(\theta) = \arg\min_{\phi(\theta') \in \text{Vert}(\mathcal{M}_N)} \|\phi(\theta') - \phi(\theta)\|.$$  

Notice that the training dynamics of the network with $N$ neurons can be characterized by

$$\frac{\partial}{\partial t} \theta_i(t) = g[\theta_i(t), \rho_i^N],$$

$$\theta_i(0) \overset{i.i.d.}{\sim} \rho_0.$$  

Here $g[\theta, \rho] = \mathbb{E}_{x, y \sim \mathcal{D}} (y - f_\sigma(x)) \nabla \theta^\sigma(\theta, x)$. We define the following coupling dynamics:

$$\frac{\partial}{\partial t} \tilde{\theta}_i(t) = g[\tilde{\theta}_i(t), \tilde{\rho}_i^\infty],$$

$$\tilde{\theta}_i(0) = \theta_i(0).$$

Notice that at any time $t$, $\tilde{\theta}_i(t)$ can be viewed as i.i.d. sample from $\tilde{\rho}_i^\infty$. We define $\tilde{\rho}_i^N(\theta) = \frac{1}{N} \sum_{i=1}^N \delta_{\tilde{\theta}_i}(\theta)$. Notice that by our definition $\theta_i = \tilde{\theta}_i(T)$ and we also define $\tilde{\theta}_i = \tilde{\theta}_i(T)$. Using the propagation of chaos argument as Mei et al. (2019) (Proposition 2 of Appendix B.2), for any $T < \infty$, for any $\delta > 0$, we have

$$\sup_{t \in [0, T]} \max_{i \in \{1, \ldots, N\}} \|\tilde{\theta}_i(t) - \theta_i(t)\| \leq \frac{C}{\sqrt{N}} \left( \sqrt{\log N} + \sqrt{\log 1/\delta} \right).$$

By Lemma 8 and the bound above, when $N$ is sufficiently large, with high probability, we have

$$\sup_{\theta \in \text{supp}(\rho_i^N)} \|\phi(\theta) - \tilde{\phi}^N(\theta)\| \leq \epsilon/2$$

$$\max_{i \in [N]} \|\tilde{\theta}_i(T) - \theta_i(T)\| \leq \frac{\epsilon}{2C},$$

where $C = \|\phi\|_{\text{Lip}}$ and

$$\tilde{\phi}^N(\theta) = \arg\min_{\theta' \in \text{supp}(\tilde{\rho}_i^\infty)} \|\phi(\theta') - \tilde{\phi}^N(\theta)\|.$$  

We denote $\tilde{\theta}_{i_0} \in \text{supp}(\tilde{\rho}_i^N)$ such that $\tilde{\phi}^N(\theta) = \phi(\tilde{\theta}_{i_0})$. It implies that

$$\sup_{\theta \in \text{supp}(\rho_i^N)} \|\phi(\theta) - \phi^N(\theta)\| \leq \sup_{\theta \in \text{supp}(\rho_i^N)} \|\phi(\theta) - \phi(\tilde{\theta}_{i_0})\|$$

$$= \sup_{\theta \in \text{supp}(\rho_i^N)} \|\phi(\theta) - \tilde{\phi}^N(\theta) + \tilde{\phi}^N(\theta) - \phi(\tilde{\theta}_{i_0})\|$$

$$= \sup_{\theta \in \text{supp}(\rho_i^N)} \|\phi(\theta) - \phi(\tilde{\theta}_{i_0}) + \phi(\tilde{\theta}_{i_0}) - \phi(\tilde{\theta}_{i_0})\|$$

$$\leq \sup_{\theta \in \text{supp}(\rho_i^N)} \|\phi(\theta) - \phi(\tilde{\theta}_{i_0})\| + \sup_{\theta \in \text{supp}(\rho_i^N)} \|\phi(\theta) - \phi(\tilde{\theta}_{i_0})\|$$

$$\leq \epsilon/2 + \max_{i \in [N]} \|\tilde{\theta}_i(T) - \theta_i(T)\| \|\phi\|_{\text{Lip}}$$

$$\leq \epsilon.$$