Sub-Optimal Local Minima Exist for Almost All Over-parameterized Neural Networks

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Abstract

Does over-parameterization eliminate sub-optimal local minima for neural network problems? On one hand, existing positive results do not prove the claim, but often weaker claims. On the other hand, existing negative results have strong assumptions on the activation functions and/or data samples, causing a large gap with positive results. It was unclear before whether there is a clean answer of “yes” or “no”. In this paper, we answer this question with a strong negative result. In particular, we prove that for deep and over-parameterized networks, sub-optimal local minima exist for generic input data samples and generic nonlinear activation. This is the setting widely studied in the global landscape of over-parameterized networks, thus our result corrects a possible misconception that “over-parameterization eliminates sub-optimal local-min”. Our construction is based on fundamental optimization analysis, and thus rather principled.

1 Introduction

It seems a common belief that recent theoretical results have provided enough evidence that all local minima are almost good. Some of the popular theoretical evidence include Choromanska et al. (2015) which essentially analyzed a special deep linear network, Kawaguchi (2016) which formally prove that deep linear networks have no sub-optimal local-min, and recent local analysis of gradient descent for ultra-wide networks Allen-Zhu et al. (2018); Du et al. (2018); Zou et al. (2018); Zou and Gu (2019). They are either restricted to linear activations or local analysis in a small region. None of these works studied the

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the global landscape of non-linear networks, and did not prove “no sub-optimal local minima” for non-linear networks.

For nonlinear networks, a few recent works have analyzed the global landscape of over-parameterized networks and some of them have proved the non-existence of sub-optimal valleys (Nguyen (2019); Nguyen et al. (2018); Venturi et al. (2018)) or bad basins (Li et al. (2018)). These works can be viewed as the extensions of the classical work Yu and Chen (1995), which claimed to have proved “no sub-optimal local minima” for 1-hidden-layer over-parameterized networks. However, later it was found by Li et al. (2018) that their proof had a cavity and therefore their claim does not hold. In short, none of the works along the line of Yu and Chen (1995) has rigorously proved the non-existence of sub-optimal local minima. Our paper aims to understand whether the lack of “no bad local-min” result is due to intrinsic barriers, or the limitation of technical skills.

There are some existing counter-examples of sub-optimal local minima under various settings (reviewed in Section 2.1), but they are restricted since they assume special data or non-smooth activations. It is still possible that a wide neural network with smooth activations and generic data, the common setting in recent positive results, admits no bad local minima. In fact, previous results already eliminate bad basins under this setting, only allowing the existence of flat local minima. It seems we are only a tiny step away from a clean result of “no sub-optimal local minima”. Perhaps surprisingly, we will show this seemingly small gap is insurmountable (without extra assumptions).

1.1 Our Contributions

We consider a supervised learning problem where the prediction is parameterized by a multi-layer neural network with hidden neurons no less than data samples. We show that highly sub-optimal local minima are quite common for over-parameterized networks. Our examples are much broader than the previous constructions of sub-optimal local minima which rely on special components.

More specifically, our contributions include: (suppose $d$ is the input dimension, and $n$ is the number of samples):

- We prove that for all analytic activation functions which are nonlinear and twice-differentiable in an arbitrarily small interval and for generic input data where $d < O(\sqrt{n})$, there exists examples such that the considered loss function contains sub-optimal local minima. This implies that under the typical settings of over-parameterized networks (e.g. Li et al. (2018); Nguyen (2019); Nguyen et al. (2018); Venturi et al. (2018); Yu and Chen (1995)), it is impossible to prove “no sub-optimal local-min” without additional assumptions.

- We show that for all realizable deep neural networks with activation that contains a linear segment, sub-optimal local minima exist for generic training samples.
• The existence of bad local-min is not universal, and there is a phase transition on the number of data samples. We show that as the number of data samples increases, there is a transition from no bad local minima to having bad local minima. In particular, if there are only one or two data samples, the considered network has no bad local minima for a wide class of activation functions. However, with three or more data samples, bad local minima exist for almost all nonlinear activations.

To the best of our knowledge, our result is the first counter-example result that covers generic non-linear activations and generic input data samples. More importantly, this result reveals the fact that “generic over-parameterized neural networks do have sub-optimal local minima”, which clarifies a misconception in recent years. It is noteworthy that our result does not imply “neural networks are always hard to train”, since there may be other ways to avoid hitting sub-optimal local minima in practice (especially after many years of tuning neural-architecture, initial point, etc.). Our goal is to reveal the ground truth of the optimization landscape under minimal assumptions.

For the convenience of readers, we summarize the existing examples and our examples in Table 1.

### Table 1: Summary of existing examples and our examples

| Reference  | Width | Over-para | Activation          | Data       |
|------------|-------|-----------|---------------------|------------|
| Auer et al.| 1     | No        | Generic\(^3\)       | Positive measure |
| Swirszcz et al. | 2 or 3 | No | Sigmoid, ReLU | Fixed |
| Zhou et al. | 1     | No        | ReLU                | Fixed     |
| Safran et al.\(^1\) | 6 to 20 | Yes | ReLU               | Gaussian |
| Venturi et al.\(^1\) | Any   | No        | \(L^2(\mathbb{R}, e^{-x^2/2})\) | Adversarial |
| Liang et al. | Any   | Yes       | \(\sigma(t) + \sigma(-t) = c\) | Fixed |
| Yun et al.  | 2     | No        | Small nonlinearity  | Fixed     |
| This paper  | Any   | Yes       | Generic nonlinear  | Generic input |

\(^1\) In these two examples, the objective function is the population risk, which is a different setting from the empirical risk minimization.

\(^2\) “Over-para” means the number of neurons in the network is no less than the number of data samples.

\(^3\) The actual requirement is that \(l(\cdot, \sigma(\cdot))\) is continuous and bounded, where \(l(\cdot)\) and \(\sigma(\cdot)\) are the loss function and the activation function separately.

### 1.2 Phase Transition and Story Behind Our Findings

We notice that the two major results on the neural-net landscape can be illustrated by the simplest 1-neuron 1-data example and thus have no phase transition. The simplest 1-neuron 1-data linear network \(F(v, w) = (1 - vw)^2\) has no sub-optimal local minima, and it turns out deep linear networks also have no sub-optimal local minima (Kawaguchi (2016)). The simplest 1-neuron 1-data non-linear network \(F(v, w) = (1 - v\sigma(w))^2\) has no bad basin, and it turns out
deep over-parameterized non-linear networks also have no bad basin \cite{Li2018}.

What about “no sub-optimal local-min” result for non-linear networks? We start from the very special case \((1 - \sigma(w))^2\) (with the second layer weight \(v\) fixed to 1). We notice that if \(\sigma\) has a “bump”, i.e., not monotone, then \(F(w) = (1 - \sigma(w))^2\) has sub-optimal local-min. Such a counter-example can easily be fixed: if \(\sigma(t)\) is strictly increasing on \(t\) then \((1 - \sigma(w))^2\) has no sub-optimal local-min. As many practical activation functions are strictly increasing (e.g., sigmoid, ELU, SoftPlus), adding a minor assumption of strictly increasing seems reasonable.

We then checked the 2-layer case \(F(v, w) = (1 - v\sigma(w))^2\). It is not straightforward to see what the landscape of this function is. For special \(\sigma\) (e.g. \(\sigma(t) = t^2\)), sub-optimal local-min exists. But this counter-example is again quite brittle, as for \(\sigma(t) = (t - 0.01)^2\) or \(\sigma(t) = t^2 + 0.01\) there is no sub-optimal local minima. With some effort, we proved that for almost all \(\sigma\) (except \(\sigma\) that achieves zero value at its local-min or local-max), the function has no sub-optimal local-min. In particular, for strictly increasing activations, \((1 - v\sigma(w))^2\) has no sub-optimal local minima. The exact conditions on the activations are not that important for our purpose, as long as it covers a broad range of activations, especially the set of strictly increasing functions. Since previous major results are extendable to more general cases, we initially made the following conjecture:

**Conjecture:** for a large set of activation functions (a superset of the set of all strictly increasing smooth functions), over-parameterized networks have no sub-optimal local-min, for generic data.

We already proved this conjecture for the case with one data point. We are able to prove it for two data points, i.e., the function \(F(v, w) = (y_1 - v\sigma(wx_1))^2 + (y_2 - v\sigma(wx_2))^2\), giving us more confidence.

Unfortunately, with \(n = 3\) samples and \(m = 3\) neurons, our proof no longer works. This failure of proof has led us to construct a counter-example to this conjecture, and later generalization of this counter-example to any number of neurons. More specifically, our counter-examples hold for almost all activation functions (in the sense that any continuous activation is arbitrarily close to an activation in our class). This is a strong negative answer to the conjecture, as disproving the conjecture only requires giving a counter-example for one strictly increasing activation and our results imply that for almost all strictly increasing activation functions (and almost all non-increasing functions as well) the conjecture fails. Finally, we note that it is impossible to show “sub-optimal local minima exist for any activations” since linear activation leads to no sub-optimal local minima. Thus our result for almost all activations is in some sense “tight”.

The paper is organized as follows. We first discuss some related works in Section 2. Then we present the network model we study in Section 3. In Section 4 we present the main results and make some discussions. The main proof idea is provided in Section 5 and the proof for the main result is presented in Section 6. We finally draw our conclusions in Section 7.
2 Related Works

2.1 Examples of Sub-optimal Local Minima

We impose mild assumptions on the network width, the activations and the data. Below, we review the counter-examples found in prior works and explain what type of bad local minima are of interest for bridging negative and positive results.

**Wide Network (Over-parameterized).** The classical work Auer et al. (1996) presented a concrete counter-example where exponentially many sub-optimal local minima exist in a single-neuron network. However, the counter-example was an unrealizable case (i.e. the network cannot fit data), and the authors proved that under the same setting, bad local minima would not exist if the network can fit data. Therefore, it is of little interest to show bad local minima exist for unrealizable cases. In order to avoid this non-interesting case, we allow arbitrary number of neurons.

**Smooth Activations.** Due to the popularity of ReLU activations, a few works showed that ReLU networks have bad local minima (e.g., Swirszcz et al. (2016), Zhou and Liang (2017), Safran and Shamir (2018), Venturi et al. (2018), Liang et al. (2018b)\(^1\)). One intuition why ReLU can lead to bad local minima is that it can create flat regions (“dead regions”) where the empirical loss remains constant. Therefore, all interior points of the flat regions are bad local minima. Intuitively, such flat regions may disappear if the activations are smooth (this is indeed proved in Liang et al. (2018b) for special data). In contrast, the existing positive results for the global landscape of over-parameterized networks are all for smooth activations, which seems to indicate that smooth activations have better landscape than non-smooth activations. Therefore, an ideal counter-example should apply to smooth activations.

**Generic Data.** There are few works (Liang et al. (2018b) and Yun et al. (2018)) that construct bad local minima for smooth activations under realizable cases, but in their examples the data points lie in a zero-measure space.\(^2\) In contrast, the existing positive results for the global landscape over-parameterized networks often assume generic data\(^3\). An ideal counter-example should apply to generic data, or at least a positive measure of data points.

These results are summarized in Table 1. Only two works Safran and Shamir (2018) and Liang et al. (2018b) have considered the over-parameterized setting, but they assume special data (Gaussian data or fixed data) and special activations (ReLU or sigmoid-like functions).

\(^1\)Safran and Shamir (2018) and Venturi et al. (2018) both provided counter-examples when the objective function is the population risk, a different setting from the empirical risk minimization considered in this paper.

\(^2\)These works have extra restrictions. Liang et al. (2018) only considers activations that satisfy \(\sigma(t) + \sigma(-t) = c, \forall t\). Yun et al. (2018) only considers a network with two neurons and three data points and thus not a wide-network setting.

\(^3\)More rigorously, a result holds for “generic” data means that except for a zero-measure set, the result holds.
2.2 Other Related Works

We discuss a few other related works in this section.

There are few works that proved no sub-optimal local minima for non-linear networks, but their settings are quite special. Liang et al. (2018b) assumes that data are special (such as linearly separable). Soltanolkotabi (2017) assumes quadratic activation, and Liang et al. (2018a) assumes a special neuron activation and an extra regularizer. These assumptions and modifications are not very practical and will not be the focus of this paper. We will study the rather general setting along the line of Yu and Chen (1995).

It is widely reported in numerical experiments that over-parameterized neural networks have nice landscape (see, e.g., Garipov et al. (2018); Geiger et al. (2018); Goodfellow et al. (2014); Livni et al. (2014); Lopez-Paz and Sagun (2018)). In particular, Draxler et al. (2018); Garipov et al. (2018) showed that in the current neural networks for image classification there are no barriers between different global minima. However, this only implies that there is no sub-optimal basin (and connected sub-level sets) and does not imply that there is no sub-optimal local minima (which can be flat). In addition, some numerical evidence on the “nice landscape” does not mean that neural network training is always easy. In fact, Dauphin et al. (2014) reported various experiments that the training can get stuck in plateaus, and He et al. (2016) also reported the plateaus in training plain deep neural networks. The difficulty in training neural networks (beyond the well-tuned image classification tasks) is still not completely understood, and we think that our negative results may help us rethink the impact of bad local minima on training neural networks.

For deep linear networks, besides the work of Kawaguchi (2016), there are a few other works that prove related results (e.g., Laurent and Brecht (2018); Lu and Kawaguchi (2017); Swirszcz et al. (2016); Zhang (2019)). For deep non-linear networks, Allen-Zhu et al. (2018); Du et al. (2018); Jacot et al. (2018); Zou et al. (2018); Zou and Gu (2019) proved that “GD can converge to global minima” for deep neural networks under the assumptions of a large number of neurons and special initialization. These works provide local analysis in a quite small region, and it is not clear whether practical training is restricted to that small neighborhood.

There have been many works on the landscape or convergence analysis of shallow neural-nets. Feizi et al. (2017); Freeman and Bruna (2016); Gao et al. (2018); Ge et al. (2018); Haefele and Vidal (2017); Panigrahy et al. (2017); Soudry and Hoffer (2017) analyzed the global landscape of various shallow networks. Brutzkus and Globerson (2017); Brutzkus et al. (2018); Du and Lee (2018); Janzamin et al. (2017); Laurent and von Brecht (2017); Li and Yuan (2017); Mei et al. (2018); Mondelli and Montanari (2018); Oymak and Soltanolkotabi (2019); Soltanolkotabi et al. (2019); Tian (2017); Wang et al. (2018); Zhong et al. (2017) analyzed gradient descent for shallow networks. Along another line, Chizat and Bach (2018); Mei et al. (2018); Rotskoff and Vanden-Eijnden (2018); Sirignano and Spiliopoulos (2018) analyzed the limiting behavior of SGD when the number of neurons goes to infinity.
3 Network Model

3.1 Network Structure

Consider a fully connected neural network with $H$ hidden layers. Assume that the $h$-th hidden layer contains $d_h$ neurons for $1 \leq h \leq H$, and the input and output layers contain $d_0$ and $d_{H+1}$ neurons, respectively. (Specifically, if there is only 1 hidden layer, we use $m$ to represent the number of neurons in the hidden layer.) Given an input sample $x \in \mathbb{R}^{d_0}$, the input of the $i$-th neuron of the $h$-th hidden layer, denoted by $z_{h,i}$, is given by

$$z_{1,i}(x) = \sum_{j=1}^{d_0} w_{1,i,j} x_j + b_{1,i}, \quad 1 \leq i \leq d_1 \tag{1a}$$

$$z_{h,i}(x) = \sum_{j=1}^{d_{h-1}} w_{h,i,j} z_{h-1,j}(x) + b_{h,i}, \quad 1 \leq i \leq d_h, \quad 2 \leq h \leq H \tag{1b}$$

where $x_j$ is the $j$-th entry of the input data, $w_{h,i,j}$ is the weight from the $j$-th neuron of the $(h-1)$-th layer to the $i$-th neuron of the $h$-th layer, $b_{h,i}$ is the bias added to the $i$-th neuron of the $h$-th layer. Let $\sigma$ be the neuron activation function. Then the output of the $i$-th neuron of the $h$-th hidden layer, denoted by $t_{h,i}$, is given by

$$t_{h,i}(x) = \sigma(z_{h,i}(x)), \quad 1 \leq i \leq d_h, \quad 1 \leq h \leq H. \tag{2}$$

Finally, the $i$-th output of the network, denoted by $t_{H+1,i}$, is given by

$$t_{H+1,i}(x) = \sum_{j=1}^{d_H} w_{H+1,i,j} t_{H,j}(x), \quad 1 \leq i \leq d_{H+1} \tag{3}$$

where $w_{H+1,i,j}$ is the weight to the output layer, defined similarly to that of the hidden layers.

Then, we define $W_h \in \mathbb{R}^{d_{h-1} \times d_h}$ as the weight matrix from the $(h-1)$-th layer to the $h$-th layer, and $b_h \in \mathbb{R}^{d_h}$ as the bias vector of the $h$-th layer. The entries of each matrix are given by

$$(W_h)_{i,j} = w_{h,i,j}, \quad (b_h)_i = b_{h,i}, \tag{4}$$

3.2 Training Data

Consider a training dataset consisting of $N$ samples. Noting that the input dimension and the output dimension are $d_0$ and $d_{H+1}$, we denote the $n$-th sample by $(x^{(n)}, y^{(n)}), \ n = 1, \cdots, N$, where $x^{(n)} \in \mathbb{R}^{d_0}, y^{(n)} \in \mathbb{R}^{d_{H+1}}$ are the input and output samples, respectively. We can rewrite all the samples in vector forms, i.e.

$$X \triangleq [x_1, x_2, \cdots, x_N] \in \mathbb{R}^{d_0 \times N} \tag{5a}$$

$$Y \triangleq [y_1, y_2, \cdots, y_N] \in \mathbb{R}^{d_{H+1} \times N}. \tag{5b}$$
With the input data given, we can represent the input and output of each hidden-layer neuron by

\[ z_{h,i,n} = z_{h,i}(x_n) \]  
\[ t_{h,i,n} = t_{h,i}(x_n) \]

for \( h = 1, 2, \cdots, H \), \( i = 1, 2, \cdots, d_h \), and \( n = 1, 2, \cdots, N \). Then, we define \( Z_h \in \mathbb{R}^{d_h \times N} \) and \( T_h \in \mathbb{R}^{d_h \times N} \) as the input and output matrix of the \( h \)-th layer with

\[ (Z_h)_{n,i} = z_{h,i,n} \]  
\[ (T_h)_{n,i} = t_{h,i,n}. \]

Similarly, we denote the output matrix by \( \hat{Y} \in \mathbb{R}^{d_{H+1} \times N} \), where

\[ (\hat{Y})_{i,n} = \hat{y}_{i,n} = t_{H+1,i}(x_n) \]

for \( i = 1, 2, \cdots, d_{H+1}, n = 1, 2, \cdots, N \).

### 3.3 Training Loss

Let \( W \) denote all the network weights, i.e.

\[ W = (W_1, b_1, W_2, b_2, \cdots, W_H, b_H, W_{H+1}) \]

In this notes, we consider the quadratic loss function to characterize the training error. That is, given the training dataset \((X, Y)\), the empirical loss is given by

\[ E(W) = ||Y - \hat{Y}(W)||^2_F. \]

Here we treat the network output \( \hat{Y} \) as a function of the network weights. Then, the training problem of the considered network is to find \( W \) to minimize the empirical loss \( E(W) \).

### 4 Main Theorems and Discussions

#### 4.1 General Example of Bad Local Minima

In this subsection, we present our main result of bad local minima. To this end, we first specify the assumptions on the data samples and the activation functions.

**Assumption 1**

\( a) \) The input dimension \( d_0 \) satisfies \( d_0^2 + d_0 < N. \)
b) The following $d_0^2 + d_0 + 1$ vectors

\[
X = \{1, X_{(1,:)}, X_{(2,:)}, \cdots, X_{(N,:)}, X_{(1,:)} \odot X_{(1,:)}, X_{(1,:)} \odot X_{(2,:)}, \cdots, X_{(i,:)} \odot X_{(j,:)}, \cdots, X_{(d_0,:)} \odot X_{(d_0,:)}\}
\tag{11}
\]

are linearly independent. Note that $X$ includes all the rows of $X$ and the Hadamard product between any two rows of $X$.

Assumption 1 holds for generic input data. That is, the input data that violates Assumption 1 only constitutes a zero-measure set in $\mathbb{R}^{d_0 \times N}$. We further note that Assumption 1 can be always achieved if we allow an arbitrarily small perturbation on the input data.

**Assumption 2** There exists $a \in \mathbb{R}$ and $\delta > 0$ such that

a) $\sigma$ is twice differentiable on $[a - \delta, a + \delta]$.

b) $\sigma(a), \sigma'(a), \sigma''(a) \neq 0$.

Assumption 2 is very mild as it only requires the activation function to have continuous and non-zero second-order derivatives in an arbitrarily small region. It holds for many widely used activations such as ELU, sigmoid, softplus, Swish, and so on. We further note that the function class specified by Assumption 2 is in fact a dense set in the space of continuous functions in the sense of uniform convergence. Therefore, by Assumption 2 we specify a “generic” class of activation functions.

**Theorem 1** Consider a multi-layer neural network with input data $X \in \mathbb{R}^{d_0 \times N}$ and $N \geq 3$. Suppose that Assumption 1 and 2 hold. Then there exists an output vector $Y \in \mathbb{R}^{d_{H+1} \times N}$ such that the empirical loss $E(W)$ has a local minimum $W$ with $E(W) > 0$.

Theorem 1 states that for generic input data and analytic activation functions, the network has a local minimum with non-zero training error regardless of width and realizability. Specifically, if the network is realizable, i.e., the empirical loss can be minimized to zero, then the considered network has bad local minima. Formally, we have the following corollary.

**Corollary 1** Consider a multi-layer neural network with input data $X \in \mathbb{R}^{d_0 \times N}$ and $N \geq 3$. Suppose that Assumption 1 and 2 hold, and the network is realizable for any output data $Y \in \mathbb{R}^{d_{H+1} \times N}$. Then there exists an output vector $Y \in \mathbb{R}^{d_{H+1} \times N}$ such that the empirical loss has sub-optimal local minima.

Corollary 1 is a rather general counter-example, which holds for generic input data and a dense class of activation functions. Although the realizability assumption seems strong, it can be easily achieved by adding a mild condition to Assumption 2. For example, Li et al. [2018] showed that for over-parameterized networks, if the activation is analytic and satisfies Assumption 2, holds, and we...
further have $\sigma^{(3)}(0), \sigma^{(4)}(0), \ldots, \sigma^{(N-1)}(0)$, then the network is realizable for generic input data regardless of the output data $Y$. Note that even with the additional conditions, the activation functions still constitute a dense set in the space of continuous functions. Besides, [Nguyen 2019], [Nguyen et al. 2018] also identify several classes of activations that guarantee the network realizability.

We next consider a type of non-linear activation functions which is “supplementary” to that specified by Assumption 2.

Assumption 3

a) There exists $a \in \mathbb{R}$ and $\delta > 0$, such that $\sigma$ is linear in $(a - \delta, a + \delta)$.

b) Each hidden layer is wider than the input layer, i.e., $d_h > d_0$ for $h = 1, 2, \ldots, H$.

c) The training data $(X, Y)$ satisfies $\text{rank}(\begin{bmatrix} X^T & 1 \end{bmatrix}) > \text{rank}(\begin{bmatrix} X^T \end{bmatrix})$.

Assumption 3 requires the activation to be at least ”partially linear”, i.e., linear in an arbitrarily small interval. Assumption 3(a) holds for many widely-used activation functions, such as piecewise-linear activations like ReLU and leaky ReLU, and linear unit activations like ELU and SeLU. Assumption 3(b) requires each hidden layer is wider than the input layer, while Assumption 3(c) holds for generic data samples $(X, Y)$.

Theorem 2

Consider a fully-connected deep neural network with $H \geq 2$ and data samples $X \in \mathbb{R}^{d_0 \times N}, Y \in \mathbb{R}^{d_{H+1} \times N}$. Suppose that Assumption 3 holds. Then the empirical loss $E(W)$ has local minimum $W$ with $E(W) > 0$.

Theorem 2 gives the condition where the network with “partially linear” activations has a local minimum with non-zero training error. Compared to Theorem 1, Theorem 2 holds for generic data samples regardless of the choice of the output data $Y$. Although the requirement that the network is wide in every layer (Assumption 3(b)) seems strong, it also indicates that the network is likely to have sufficient representation power. Specifically, if the network is realizable, similar to Corollary 1, the considered network has bad local minima:

Corollary 2

Consider a fully-connected deep neural network with $H \geq 2$ and data samples $X \in \mathbb{R}^{d_0 \times N}, Y \in \mathbb{R}^{d_{H+1} \times N}$. Suppose that Assumption 3 holds and that the network is realizable for $(X, Y)$. Then the empirical loss $E(W)$ has sub-optimal local minima.

4.2 No Bad Local-Min for Small Data Set

The understanding of local minima for neural networks is divided. On one hand, many researchers thought over-parameterization eliminates bad local minima and thus the results of this paper a bit surprising. On the other hand, experts may think the existence of bad local-min is not surprising since symmetry causes bad local minima. More specifically, one common intuition is that if there are
two distinct global minima with barriers in between, then bad local minima can arise in the paths connecting these two global minima. However, this intuition is not rigorous, since it is possible that all points between the two global minima are saddle points. For instance, \( F(v, w) = (1 - vw)^2 \) contains two branches of global minima in the positive orthant and the negative orthant, but on the paths connecting the two branches, there are no other local minima but only saddle points.

In this subsection, we rigorously prove that if the number of data is no more than 2, then we can prove no bad local-min for a large class of activations (though not a dense set of activations for two data samples). This reveals an interesting phenomenon that the size of training data will also affect the existence of local minima.

To illustrate this phenomenon, we consider a 1-hidden-layer neural network without bias and let both the input and the output data dimension be one. As we are studying a simple network, we adopt a simplified version notations. Specifically, We represent the network output as

\[
\hat{y}(x) = \sum_{i=1}^{m} v_i \sigma(w_i x),
\]

where \( m \) is the number of neurons in the hidden layer and \( x, y, \hat{y} \in \mathbb{R}^N \) are the input samples, the true output samples and the output vector by the network, respectively. We also denote \( v, w \in \mathbb{R}^m \) as the weight vectors, where \( v_i \) is the weight from the \( i \)-th hidden layer neuron to the output neuron, and \( w_i \) is the weight from the input neuron to the \( i \)-th hidden layer neuron.

In the following, we will show that if the network has only one or two neurons, bad local minima do not exist for a wide range of network settings. This finding, together with Theorem 1, characterizes a phase transition from no bad local minima to having bad local minima.

First, if the network has one data sample and one neuron, we give the sufficient and necessary condition for the existence of sub-optimal local minima. This result shows that networks with one data sample have no bad local minima for almost all continuous activations.

**Assumption 4** The activation function \( \sigma(t) \) is continuous. Further, for any \( t \in \mathbb{R} \), if \( \sigma(t) = 0 \), \( t \) is not a local minimum or local maximum of \( \sigma \).

Assumption 4 identifies a class of functions without local minimum or maximum with zero value, which constitute a dense set in the space of activation functions.

**Theorem 3** Consider a 1-hidden-layer neural network with \( m = N = 1 \) and the input data \( x \neq 0 \). Then the empirical loss \( E(w, v) \) has no bad local minima if and only if Assumption 4 holds.

If the network has two data samples and two hidden-layer-neurons, we also establish a theorem that guarantees the non-existence of sub-optimal bad local minima.
Assumption 5 The activation function $\sigma$ is analytic and satisfies the following conditions:

1. $\sigma(0) \neq 0$;
2. $\sigma'(t) \neq 0$, $\forall t \in \mathbb{R}$;
3. $\frac{\sigma(\lambda t_1)}{\sigma'(\lambda t_1)} \neq \frac{\sigma(\lambda t_2)}{\sigma'(\lambda t_2)}$, $\forall t_1, t_2 \neq 0$, $t_1 \neq t_2$, $\lambda \in \mathbb{R}$.

Assumption 5 holds for a wide class of strictly increasing/decreasing analytic functions, e.g., exponential functions, but these functions are not dense in the space of continuous activations.

Theorem 4 Consider a 1-hidden-layer neural network with $m = N = 2$ and input data $x_1 \neq x_2$. Suppose that Assumption 5 holds. Then the empirical loss $E(w, v)$ has no sub-optimal local minima.

Theorem 3 and 4 only consider the case of $m = N \leq 2$. However, we note that the conclusions of no bad local minima directly generalize to the case with $m \geq N$ and $N \leq 2$. The reason is that if we have $m > N = 2$ or $m > N = 1$, any sub-network with exactly $N$ neurons is realizable and has no bad local minima. Then, from any sub-optimal point we can find a strictly decreasing path to the global minimum by only optimizing any of such sub-networks. Therefore, the original network also has no sub-optimal local minima.

Our results on small dataset are somewhat counter-intuitive. In general, to determine whether sub-optimal local minima exist is a challenging task for networks of practical sizes. A natural idea is to begin with a simplest toy model, say, networks with one or two data samples. One may expect that the result on the toy model can be extended to the general case. However, we see that this is not true for even 1-hidden-layer networks.

If the training set has only one or two data samples, and the activation meets some special requirements, over-parameterized networks have no bad local minima. This result is quite positive, echoing with other positive results on over-parameterized neural networks [Nguyen (2019); Nguyen et al. (2018); Venturi et al. (2018); Yu and Chen (1995)]. Then, a direct conjecture is that, as the size of training set grows, the network still contains no bad local minima if appropriate conditions are posted on the activation function. However, our main result shows that this is not true. In fact, once the size of dataset exceeds two, bad local minima exist for almost all over-parameterized and realizable networks. However, it turns out that the results on toy models do not reveal the true landscape property of general models, and even convey misleading information.

5 Proof Idea

In this section, we use a 1-hidden-layer example to demonstrate the key idea in finding sub-optimal local minima in neural networks. In particular, we adopt the settings in Section 4.2 and prove the following theorem.
Theorem 5 Consider a 1-hidden-layer neural network with input data $x \in \mathbb{R}^N$ and $N \geq 3$. Suppose that the following assumptions hold:

- The input data samples are distinct from each other, i.e., $x_i \neq x_j$ for any $i \neq j$.
- The activation function $\sigma$ is analytic and satisfies $\sigma(0), \sigma'(0), \sigma''(0) \neq 0$.

Then there exists an output vector $y \in \mathbb{R}^N$ such that the empirical loss has a local minimum $(w, v)$ with $E(w, v) > 0$.

The proof of Theorem 5 consists of three steps.

**Step 1:** Decomposing the difference of empirical loss.

Consider an arbitrarily perturbation from $(w, v)$ to $(w', v') = (w + \Delta w, v + \Delta v)$. Denote $\hat{y}' = v'^\top \sigma(w'x^\top)$, then the objective function after perturbation is given by $E(w', v') = \|y - \hat{y}'\|_2^2$. The following lemma provides a sufficient condition for $E(w', v') \geq E(w, v)$.

**Lemma 1** If $(y - \hat{y})^\top (\hat{y}' - \hat{y}) \leq 0$, then $E(w', v') \geq E(w, v)$.

**Proof:** After the perturbation, we have

$$E(w', v') - E(w, v) = \|y - \hat{y}'\|_2^2 - \|y - \hat{y}\|_2^2 = -2(y - \hat{y})^\top (\hat{y}' - \hat{y}) + \|\hat{y}' - \hat{y}\|_2^2.$$ 

Note that $\|\hat{y}' - \hat{y}\|_2^2$ is always non-negative. Therefore, $(y - \hat{y})^\top (\hat{y}' - \hat{y}) \leq 0$ implies $E(w', v') \geq E(w, v)$. We complete the proof.

Since we can arbitrarily choose $y$, equivalently we can arbitrarily choose $\Delta y \triangleq y - \hat{y}$. From Lemma 1 what remains is to find $\Delta y^*, w^*$, and $v^*$ such that $(\Delta y, \hat{y}' - \hat{y}) \leq 0$ holds for any $(w', v')$ in a small neighbourhood of $(w, v)$.

**Step 2:** Expand $\hat{y}' - \hat{y}$ to the second-order.

Note that

$$(\hat{y}' - \hat{y})^\top = (w + \Delta w)^\top \sigma((w + \Delta w)x^\top) - v^\top \sigma(wx^\top) = \sum_{i=1}^{m} (v_i + \Delta v_i) \sigma((w_i + \Delta w_i)x_i) - \sum_{i=1}^{m} v_i \sigma(w_i x_i^\top).$$

We define

$$\partial z_i = [x_1 \sigma'(w_i x_1), \cdots, x_N \sigma'(w_i x_N)]^\top, \quad (13a)$$

$$\partial^2 z_i = \begin{bmatrix} \frac{1}{2} x_1^2 \sigma''(w_i x_1), & \cdots, & \frac{1}{2} x_N^2 \sigma''(w_i x_N) \end{bmatrix}^\top. \quad (13b)$$

Then, by Taylor expansion, we can rewrite $\sigma((w_i + \Delta w_i)x_i^\top)$ as

$$\sigma((w_i + \Delta w_i)x_i^\top) = [\sigma((w_i + \Delta w_i)x_1), \cdots, \sigma((w_i + \Delta w_i)x_N)] = z_i^\top + \Delta w_i \partial z_i^\top + (\Delta w_i)^2 \partial^2 z_i^\top + o((\Delta w_i^2)^\top) \quad (14)$$
for $i = 1, 2, \cdots, m$, where $\mathbf{o}(\cdot)$ denotes an infinitesimal vector with
\[
\mathbf{o}(t) = [o_1(t), o_2(t) \cdots, o_N(t)]^\top \in \mathbb{R}^N
\] (15a)
\[
\lim_{t \to 0} \frac{\|\mathbf{o}(t)\|_2}{|t|} = 0
\] (15b)

Thus we can represent $\hat{y}' - \hat{y}$ as
\[
\hat{y}' - \hat{y} = \sum_{i=1}^{m} (v_i + \Delta v_i) \left[ z_i + \partial z_i + \partial^2 z_i + \mathbf{o}(\Delta w_i^2) \right] - \sum_{i=1}^{m} v_i z_i
\]
= \sum_{i=1}^{m} (\Delta v_i z_i + v_i \Delta w_i \partial z_i) + \sum_{i=1}^{m} [\Delta v_i \Delta w_i \partial z_i + v_i (\Delta w_i)^2 \partial^2 z_i] + \mathbf{o}(\|\Delta w\|_2^2).

For simplicity, denote $\Delta y = y - \hat{y}$. Combining Step 1 and Step 2, we rewrite the desired inequality $\langle y - \hat{y}, \hat{y}' - \hat{y} \rangle \leq 0$ as
\[
0 \geq \langle y - \hat{y}, \hat{y}' - \hat{y} \rangle = \sum_{i=1}^{m} \Delta v_i (\Delta y, z_i) + \sum_{i=1}^{m} (\Delta v_i \Delta w_i + v_i \Delta w_i) \langle v^p, \partial z_i \rangle
\]
+ \sum_{i=1}^{m} v_i (\Delta w_i)^2 \langle \Delta y, \partial^2 z_i \rangle + \mathbf{o}(\|\Delta w\|_2^2, \Delta y).

**Step 3:** Solve a linear system to satisfy equation (16).

The final step is to select proper $w^*$, $v^*$ and $y^*$ such that equation (16) holds. Note that in (16), the sign of the second-order term is not related to $\Delta v$ or $\Delta w$. Therefore, we can make $\langle \Delta y, z_i \rangle = \langle v^p, \partial z_i \rangle = 0$ and $v_i \cdot (\Delta y, \partial^2 z_i) < 0$ for $i = 1, \cdots, m$ so that the non-positive terms dominate the right hand side of (16).

Specifically, let $w^* = 0$, then $z_1 = \cdots = z_m$, and the right hand side of (16) becomes
\[
\left( \sum_{i=1}^{m} \Delta v_i \right) \cdot (\Delta y, z_1) + \left( \sum_{i=1}^{m} (\Delta v_i \Delta w_i + v_i \Delta w_i) \right) \cdot \langle v^p, \partial z_1 \rangle
\]
+ \left( \sum_{i=1}^{m} v_i (\Delta w_i)^2 \right) \cdot \langle \Delta y, \partial^2 z_1 \rangle + \mathbf{o}(\|\Delta w\|_2^2, \Delta y).

To this end, we introduce a very simple lemma.

**Lemma 2** Given $z_1, z_2, z_3 \in \mathbb{R}^N$ where $N \geq 3$. Assume that $z_3$ is not a linear combination of $z_1$ and $z_2$, then there exists $y \in \mathbb{R}^N$ such that $y^\top z_1 = y^\top z_2 = 0$ and $y^\top z_3 \neq 0$.

**Proof:** Let $W = \text{span}\{z_1, z_2\}$. Decompose $z_3$ into $z_3 = u + v$, where $u \in W$ and $v \in W^\perp$. Since $z_3$ is not a linear combination of $z_1$ and $z_2$, $v \neq 0$, so $v^\top z_3 \neq 0$. Moreover, $u^\top z_1 = u^\top z_2 = 0$. Taking $y = v$ completes the proof. \square
Since Assumption A2 holds, the first 3-by-3 submatrix of \[
\begin{bmatrix}
z_1^T \\
\partial z_1^T \\
\partial^2 z_1^T
\end{bmatrix}
\] has the form
\[
\begin{bmatrix}
\sigma(0) & \sigma(0) & \sigma(0) \\
x_1 \sigma'(0) & x_2 \sigma'(0) & x_3 \sigma'(0) \\
x_1^2 \sigma''(0) & x_2^2 \sigma''(0) & x_3^2 \sigma''(0)
\end{bmatrix},
\]
is a Vandermonde matrix with each row scaled by a non-zero constant. Thus, \(\partial^2 z_1\) is not a linear combination of \(z_1\) and \(\partial z_1\). According to Lemma 2, there exists \((\Delta y^*) \in \mathbb{R}^N\) such that \(\langle (\Delta y^*), z_i \rangle = \langle (\Delta y^*), \partial z_i \rangle = 0\) and \(\langle (\Delta y^*), \partial^2 z_i \rangle \neq 0\). Let \(y^* = \hat{y} + (\Delta y)^*\) and \(v_i^* = -\text{sgn}(\langle (\Delta y)^*, \partial^2 z_i \rangle)\) for all \(1 \leq i \leq m\). Now expression (17) turns into
\[
\left( \sum_{i=1}^{m} v_i (\Delta w_i)^2 \right) \cdot \langle \Delta y, \partial^2 z_1 \rangle + \langle o(\|\Delta w\|^2), \Delta y \rangle.
\] (18)
If \(\Delta w = 0\) for all \(i = 1, \ldots, m\), (18) is constant 0. If \(\Delta w \neq 0\), \(\sum_{i=1}^{m} v_i (\Delta w_i)^2 \cdot \langle \Delta y, \partial^2 z_1 \rangle\) is strictly negative. Moreover, it dominates \(\langle o(\|\Delta w\|^2), \Delta y \rangle\) for sufficiently small \(\Delta w\). Therefore, (18) is always non-positive, which implies that (16) always holds. So we have shown that \((w^*, v^*)\) is a local minimum with non-zero value when the output samples are selected as \(y^*\). The proof is complete.

We provide some concluding remarks about this proof. Seeing through the proof procedure, what is actually done is expressing the difference of the empirical loss into a second-order Taylor expansion. After removing some quadratic terms, we find that the remaining terms have simple expression. In particular, the signs of the second-order terms are easy to control despite the existence of perturbation. Therefore, we control the sign of the remaining terms by zeroing out the zero-order and first-order terms so that the second-order terms dominate the whole expression. Specifically, the zeroing-out process is achieved by solving linear systems.

Although deep neural networks seem to have much more complicated expressions, the same procedure can be utilized. It is also noteworthy that adding bias does not influence the proof technique, nor does it influence the phase transition phenomenon.

6 Proof of Theorem 1

6.1 Preliminaries

For convenience, we first introduce the following notations. For \(1 \leq h_1 \leq h_2 \leq H\), let
\[
W_{[h_1:h_2]} = (W_{h_1}, b_{h_1}, W_{h_1+1}, b_{h_1+1}, \ldots, W_{h_2}, b_{h_2})
\] (19)
be the weights from the \(h_1\)-th layer to the \(h_2\)-th layer and
\[
W_{[h_1:(H+1)]} = (W_{h_1}, b_{h_1}, W_{h_1+1}, b_{h_1+1}, \ldots, W_{H}, b_{H}, W_{H+1})
\] (20)
be the weights from the \( h_1 \)-th layer to the \((H + 1)\)-th layer. Then for the \( i \)-th neuron in the \( h \)-th hidden layer, the input and output is a function of \( W_{[1:h]} \) and \( x_n \), written as \( t_{h,i}(W_{[1:h]}, x_n) \) and \( z_{h,i}(W_{[1:h]}, x_n) \), respectively.

For two weight settings \( W \) and \( W' \), we denote
\[
\tilde{W}' = (W_1, b'_1, W'_2, b'_2, \ldots, W'_H, b'_H, W'_{H+1})
\]  
(21)
where the weights to the first hidden layer are picked from \( W \), while the bias to the first hidden layer and the remaining weights and bias are all from \( W' \).

### 6.2 Local Minimum Construction

We construct the weights as follows.

1. \( W_1 = 0 \);
2. \( w_{h,i,j} > 0, \ h = 2, \cdots, H + 1 \quad i = 1, \cdots, d_h, \quad j = 1, \cdots, d_{h-1} \);
3. \( b_1 = a \cdot 1 \);
4. \( b_{h,i} = a - \sigma(a) \sum_{j=1}^{d_{h-1}} w_{h,i,j}, \ h = 2, \cdots, H, \quad i = 1, \cdots, d_h \).

We would like to make some comments on the construction above.

First, we see that in (1), the weights to the first hidden layer are set to be zero, and in (2) the weights to other hidden layers are arbitrary values with the same sign as \( \sigma'(a) \), and the weights to all other layers are arbitrary positive values. This implies that there exists \( \delta_1 > 0 \) such that for any \( W' \in B(W, \delta_1) \), conditions (2) are also satisfied by \( W' \), i.e.
\[
w'_{h,i,j} > 0, \quad h = 2, \cdots, H + 1, \quad \forall i, j \quad (22a)
\]

Second, It can be readily verified that with bias satisfying (3) and (4), for any input sample the input to all hidden-layer neurons is \( a \), so we have \( t_{h,i,n} = \sigma(a) \) for all \( h, i, n \). Notice that \( \sigma \) is twice differentiable on \([a - \delta, a + \delta]\). Therefore there exists \( \delta_2 > 0 \) such that for any \( W' \in B(W, \delta_2) \), the input of each hidden neuron is within \([a - \delta, a + \delta]\). Further, the signs of \( \sigma'(z_{h,i}(W')) \), \( \sigma'(z_{h,i}(W')) \), and \( \sigma''(z_{h,i}(W')) \) do not change, i.e.
\[
z_{h,i}(W') \in (a - \delta, a + \delta) \quad (23a)
\]
\[
t_{h,i}(W') * \sigma(a) = \sigma(z_{h,i}(W')) * \sigma(a) > 0 \quad (23b)
\]
\[
\sigma'(z_{h,i}(W')) * \sigma'(a) > 0 \quad (23c)
\]
\[
\sigma''(z_{h,i}(W')) * \sigma''(a) > 0 \quad (23d)
\]
for \( h = 1, \cdots, H \), and \( i = 1, \cdots, d_h \). Then, within \( B(W, \delta_2) \), the input and output of each neuron are twice differentiable functions with respect to the weights.

In the remaining proof, whenever we consider a weight perturbation \( W' \) around \( W \), we always assume \( W' \in B(W, \min\{\delta_1, \delta_2\}) \).
Now, let $\hat{Y}(W)$ be the resulting network output of the constructed weights. We then pick the training output data $Y$ such that each row of $\Delta Y \equiv \hat{Y}(W) - Y$ satisfies

\begin{align}
\langle \Delta Y_{(i,:)} , {1} \rangle &= 0 \quad (24a) \\
\langle \Delta Y_{(i,:)} , X_{(j,:)} \rangle &= 0 \quad (24b) \\
\langle \Delta Y_{(i,:)} , X_{(j,:)} \circ X_{(j',:)} \rangle &= 0 \quad (24c) \\
[\sigma'(a)]^{H-1} \sigma''(a) \langle \Delta Y_{(i,:)} , X_{(j,:)} \circ X_{(j,:)} \rangle &> 0 \quad (24d)
\end{align}

For any $i = 1, 2, \ldots, d_{H+1}$ and $j, j' = 1, 2, \ldots, d_0$ with $j \neq j'$.

To guarantee the existence of such $Y$, we present the following lemma.

**Lemma 3** Consider a fully-connected deep neural network with $H \geq 2$. Suppose that Assumption 1 hold. Then for any $W$, there exists $Y$ satisfying (24).

To prove Theorem 1, what remains is to show that for the constructed $W$ and $Y$, $W$ is a local minimum of the empirical loss with $E(W) > 0$.

### 6.3 Perturbation Direction

Consider a small perturbation $W'$ around the constructed $W$. The resulting difference of the training loss is given by

$$
E(W') - E(W) = ||\hat{Y}(W') - Y||_F^2 - ||\hat{Y}(W) - Y||_F^2 \\
= 2 \langle \Delta Y, \hat{Y}(W') - \hat{Y}(W) \rangle_F + ||\hat{Y}(W') - \hat{Y}(W)||_F^2 \quad (25)
$$

Therefore $E(W') - E(W) \geq 0$ if

$$
\langle \Delta Y, \hat{Y}(W') - \hat{Y}(W) \rangle_F \geq 0. \quad (26)
$$

We can further decompose $\hat{Y}(W') - \hat{Y}(W)$ as

$$
\hat{Y}(W') - \hat{Y}(W) = \hat{Y}(\bar{W}') - \hat{Y}(W) + \hat{Y}(W') - \hat{Y}(\bar{W}') \quad (27)
$$

To prove that $W$ is a local minimum, it suffices to show that for any $W'$ that is sufficiently close to $W$, we have

\begin{align}
\langle \Delta Y, \hat{Y}(W') - \hat{Y}(W) \rangle_F &\geq 0 \quad (28a) \\
\langle \Delta Y, \hat{Y}(W') - \hat{Y}(W') \rangle_F &\geq 0 \quad (28b)
\end{align}

We first show that, for the constructed $W$ and any $W'$, (28a) holds.

In fact, if $W_1 = 0$, each network output $t_{H+1,i}(x)$ is invariant to the input vector $x$. Therefore, we have

\begin{align}
\hat{y}_{i,1}(W) &= \hat{y}_{i,2}(W) = \cdots = \hat{y}_{i,N}(W) \quad (29a) \\
\hat{y}_{i,1}(\bar{W}') &= \hat{y}_{i,2}(\bar{W}') = \cdots = \hat{y}_{i,N}(\bar{W}') \quad (29b)
\end{align}

17
for \(i = 1, 2, \cdots, d_{H+1}\). Thus, for \(W\) and \(\tilde{W}'\), each row of the network output matrix can be written as

\[
\hat{Y}(i,:) = \tilde{y}_{i,1}(W) \cdot 1 \\
\hat{Y}(i,:)(\tilde{W}') = \tilde{y}_{i,1}(\tilde{W}') \cdot 1
\] (30a) (30b)

and from (24a) we have

\[
\langle \Delta Y, \hat{Y}(W'') - \hat{Y}(W) \rangle_F = 0
\]

implying that (28a) is satisfied.

Then we present the following lemma.

**Lemma 4** Consider a fully-connected deep neural network with \(H \geq 2\). Suppose that Assumption 1 and 2 hold. Then for the \(W\) and \(Y\) constructed in Section 6.2, there exists \(\delta_3 > 0\) such that for any \(W' \in B(W, \delta_3)\)

\[
\langle \Delta Y, \hat{Y}(W') - \hat{Y}''(W') \rangle_F \geq 0
\] (32)

where the equality holds if and only if \(\|W'_1 - W_1\|^2_F = 0\).

Therefore, (28b) is satisfied by \(W'\) that is sufficiently close to \(W\). We complete the proof.

### 7 Conclusion

In this paper, we studied the existence of sub-optimal local minima in nonlinear neural networks. Specifically, we show that bad local minima exist for over-parameterized networks with almost all analytic activations. We also discover a transition of the landscape influenced by the size of training data set. Our result solves a long-standing question of “whether sub-optimal local minima exist in general neural networks”, and the answer is somewhat astonishingly negative. Nevertheless, combining with other positive results, we believe that this work reveals the exact landscape of over-parameterized neural networks, which is not as nice as people generally think but much better than general non-convex functions. This work also provides a future research direction of how to avoid such sub-optimal local minima effectively in a general setting during the training process, and calls for a deeper understanding of the empirical efficiency of training neural networks.
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A Proof of Theorem 3

Before we start the proof, note that $\sigma(t) \equiv 0$ does not satisfy the condition, so there must exist some $t$ such that $\sigma(t) \neq 0$. Since $x \neq 0$, let $w = \frac{x}{\hat{y}}$ and $v = \frac{y}{\sigma(t)}$, then $\hat{y} = w\sigma(wx) = \sigma(t) = y$ and $E(\theta) = 0$. This implies that the network is always realizable.

We first prove the sufficiency of the condition. Due to the realizability of the network, we now only need to show that all $\theta$ such that $\hat{y} \neq y$ are not local minima. Consider any $\theta = (v, w)$ such that $\hat{y} = v\sigma(wx) \neq y$. Note that $E(\theta) = (y - \hat{y})^2 = (y - v\sigma(wx))^2$ is convex in $v$. 
• If $\sigma(wx) \neq 0$, then there is a strict decreasing path from $(v, w)$ to $(v', w)$ where $v' = \frac{-y}{\sigma(wx)}$, so $\theta = (v, w)$ is not a local minimum.

• If $\sigma(wx) = 0$, then $\hat{y} = v\sigma(wx) = 0$. Since $\theta$ is not a global minimum, $y \neq \hat{y} = 0$. Due to the condition, $wx$ is neither a local maximum nor local minimum of $\sigma$. Therefore, for any $\delta > 0$, there exists $w_1, w_2 \in B(v, \delta)$ such that $\sigma(w_1x) > 0, \sigma(w_2x) < 0$. Further, for any $\delta > 0$, there exists $v' \in B(v, \delta)$ such that $v' \neq 0$. Thus there is exactly one positive and one negative value in $v'\sigma(w_1x)$ and $v'\sigma(w_2x)$. Take the one with the same sign as $y$, we obtain a smaller objective value in the neighborhood $B((v, w), 2\delta)$. This means that $(v, w)$ is not a local minimum.

Combining the two cases above we finish the sufficiency part of the proof.

For the necessity part, we construct a sub-optimal local minima when the condition does not hold. Without losing genoristy, assume that $y \neq 0$, $t_0$ is a local minimum and $\sigma(t_0) = 0$. Take $w_0 = \frac{\partial L}{\partial y}$ and any $v_0$ such that $v_0y < 0$. Then, $\hat{y}_0 = v_0\sigma(t_0) = 0$. On the other hand, for any $(v, w)$ in the neighborhood of $(v_0, w_0)$, $\sigma(wx) \geq 0$ since $t_0$ is a local minimum of $\sigma$. Moreover, since $v$ has the same sign with $v_0$, we have $v\sigma(wx) \cdot y \leq 0$. Therefore, $(y - v\sigma(wx))^2 \geq y^2 = (y - \hat{y})^2$ for any $(v, w)$ in the neighborhood of $(v_0, w_0)$, which means that $\theta_0 = (v_0, w_0)$ is a local minimum. Moreover, since $y \neq 0 = \hat{y}_0$, it is a sub-optimal local minimum. The necessity part is completed.

Therefore the condition above is a necessary and sufficient condition for non-existence of sub-optimal local minima in the single-neuron networks.

## B Proof of Theorem 4

For simplicity, we denote the weight parameter by $\theta = (w, v)$. Although in this paper we only consider quadratic loss, Theorem 4 also holds for any convex and differentiable loss function. Hence we provide a more general proof here. Specifically, for given data $(x, y)$, the empirical loss is given by

$$E(\theta) = L(\hat{y}(\theta))$$

where $L : \mathbb{R}^N \rightarrow \mathbb{R}$ is a convex and differentiable function.

We first present a useful lemma.

**Lemma 5** Consider a convex and differentiable function $L(\cdot)$. Suppose that $\hat{y}$ is not a global minimum of $L(\cdot)$. Then for any $\epsilon > 0$ there exists $\delta > 0$, such that for any $\hat{y}' \in B_\epsilon(\hat{y}, \delta)$ and $\langle \hat{y}' - \hat{y}, -\nabla L(\hat{y}) \rangle > \epsilon \|\hat{y}' - \hat{y}\|_2$, we have $L(\hat{y}') < L(\hat{y})$.

**Proof:** Note that $\nabla L(\hat{y}) \neq 0$ since $\hat{y}$ is not a global minimum. By Taylor expansion of $L(\hat{y})$ we have

$$L(\hat{y}') = L(\hat{y}) + \langle \hat{y}' - \hat{y}, \nabla L(\hat{y}) \rangle + o(\|\hat{y}' - \hat{y}\|_2).$$ (34)
For any $\epsilon > 0$, there exists $\delta > 0$ such that $|o(||\hat{y}' - \hat{y}||_2)| < \epsilon ||\hat{y}' - \hat{y}||_2$ for any $\hat{y}' \in B_o(\hat{y}, \delta)$. Then for any $\hat{y}' \in B_o(\hat{y}, \delta)$ and $\langle \hat{y}' - \hat{y}, -\nabla L(\hat{y}) \rangle > \epsilon ||\hat{y}' - \hat{y}||_2$, we have
\[
\langle \hat{y}' - \hat{y}, -\nabla L(\hat{y}) \rangle < -\epsilon ||\hat{y}' - \hat{y}|| < -o(||\hat{y}' - \hat{y}||_2)
\] (35)
and therefore
\[
L(\hat{y}') - L(\hat{y}) < -\epsilon ||\hat{y}' - \hat{y}||_2 + o(||\hat{y}' - \hat{y}||_2) < 0.
\] (36)
We complete the proof.

Consider a weight parameter $\theta$ that is not a global minimum. This implies that the corresponding $\hat{y}$ is not a global minimum of the loss function $L(\cdot)$, and $\nabla L(\hat{y}) \neq 0$. In what follows, we show that there exists a perturbation of $\theta$, which can be made arbitrarily small, such that the empirical loss decreases. This implies that $\theta$ cannot be a local minimum. Specifically, for any $\epsilon > 0$, we prove that there exists $\theta' = (w', v') \in B_o(\theta, \epsilon)$ such that $E(\theta') < E(\theta)$.

Denote
\[
Z = \sigma(wx^\top) \in \mathbb{R}^{2 \times 2}.
\] (37)
Then $z_1^\top$ and $z_2^\top$ are the first and the second rows of $Z$, respectively.

If $v = 0$, then $\hat{y} = 0$. In this case any perturbation of $w$ will not change $\hat{y}$, and hence will not change the empirical loss. Note that the considered network is over-parameterized with $\sigma(0), \sigma'(0) \neq 0$. Following the conclusion in Li et al. (2018), there exists a perturbation of $w$, which can be made arbitrarily small, such that there exists a strictly decreasing path from the perturbed point to the global minimum of the loss function, i.e., zero empirical loss. This implies that there exists $\theta' \in B_o(\theta, \epsilon)$ such that $E(\theta') < E(\theta)$.

If $v \neq 0$, without loss of generality we assume $v_1 \neq 0$. Regarding the direction of $z_1$, we discuss the following two cases.

**Case 1:** $\langle z_1, \nabla L(\hat{y}) \rangle \neq 0$. In this case we can achieve a smaller empirical loss by only perturbing $v$. Let $a = \langle z_1, \nabla L(\hat{y}) \rangle$ and $v' = (v_1 - \lambda \text{sign}(a), v_2)^\top$, then
\[
\hat{y}' - \hat{y} = -\lambda \text{sign}(a)z_1^\top.
\] (38)
By Lemma\ref{lemma:gradient} there exists $\delta > 0$ such that for any $\hat{y}' \in B_o(\hat{y}, \delta)$, if
\[
\langle (\hat{y}' - \hat{y})^\top, -\nabla L(\hat{y}) \rangle > \frac{|a|}{2||z_1||_2}||\hat{y} - \hat{y}_0||_2
\] (39)
then $L(\hat{y}') < L(\hat{y})$.

By letting
\[
\lambda < \min \left\{ \frac{\delta}{||z_1||_2}, \epsilon \right\}
\] (40)

24
we have \( ||\hat{y}' - \hat{y}||_2 = \lambda ||z_1||_2 < \delta \), and

\[
\langle (\hat{y}' - \hat{y})^T, -\nabla L(\hat{y}) \rangle = \lambda \text{sign}(a) \langle z_1, \nabla L(\hat{y}) \rangle = \lambda |a| \tag{41a}
\]

\[
= \frac{|a|}{||z_1||_2} ||\hat{y}' - \hat{y}||_2 \tag{41b}
\]

\[
> \frac{|a|}{2||z_1||_2} ||\hat{y}' - \hat{y}||_2. \tag{41c}
\]

Then \( L(\hat{y}') < L(\hat{y}) \). Note that \( ||v' - v||_2 = \lambda < \epsilon \), and hence the perturbation is within \( B_\epsilon(\theta, \epsilon) \).

**Case 2:** \( \langle z_1, \nabla L(\hat{y}) \rangle = 0 \). In this case we show that we can decrease the empirical loss by only perturbing \( w \). Define

\[
\partial z_1 = [x_1 \sigma'(w_1 x_1), x_2 \sigma'(w_1 x_2)]^T \in \mathbb{R}^{2 \times 1}. \tag{42}
\]

We first show that \( \langle \partial z_1, \nabla L(\hat{y}) \rangle \neq 0 \). Note that \( x_1 \neq x_2 \) and from Assumption \( 5 \) \( \sigma'(w_1 x_1), \sigma'(w_1 x_2) \neq 0 \). Hence \( \partial z_1 \neq 0 \). Also, we can show that \( z_1 \neq 0 \). This is because if \( w_1 = 0 \), \( \sigma(w_1 x_1) = \sigma(w_1 x_2) \neq 0 \), and if \( w_1 \neq 0 \), \( \sigma(w_1 x_1) \neq \sigma(w_1 x_2) \). Now, since \( z_1, \partial z_1 \neq 0 \), the third point of Assumption \( 5 \) implies that \( z_1 \) is linearly independent of \( \partial z_1 \), and therefore \( \text{span}\{z_1, \partial z_1\} = \mathbb{R}^2 \). As \( \langle z_1, \nabla L(\hat{y}) \rangle = 0 \), we must have \( \langle \partial z_1, \nabla L(\hat{y}) \rangle \neq 0 \).

Denote

\[
a = \langle \partial z_1, \nabla L(\hat{y}) \rangle, \quad b = \langle x, \nabla L(\hat{y}) \rangle. \tag{43}
\]

Let \( w' = (w_1 + \Delta w_1, w_2) \) and \( v' = v \) where \( \Delta w_1 \neq 0 \). We have

\[
\hat{y}' - \hat{y} = v_1 (\sigma(w_1 x_1 + \Delta w_1 x_1) - \sigma(w_1 x_1), \sigma(w_1 x_2 + \Delta w_1 x_2) - \sigma(w_1 x_2))
\]

\[
= v_1 (\Delta w_1 x_1 \sigma'(w_1 x_1) + o(\Delta w_1 x_1), \Delta w_1 x_2 \sigma'(w_1 x_2) + o(\Delta w_1 x_2)) \tag{44}
\]

\[
= v_1 \Delta w_1 \partial z_1^T + o(\Delta w_1) x^T.
\]

and

\[
\langle (\hat{y}' - \hat{y})^T, \nabla L(\hat{y}) \rangle = v_1 \Delta w_1 a + o(\Delta w_1) b. \tag{45}
\]

Note that \( v_1, a, \Delta w_1, ||\partial z_1||_2 \neq 0 \). From \((44)\), there exists \( \delta_1 \) such that

\[
||\hat{y}' - \hat{y}||_2 \leq ||v_1 \Delta w_1 \partial z_1||_2 + ||o(\Delta w_1) x||_2
\]

\[
< 2|v_1 \Delta w_1| \cdot ||\partial z_1||_2 \tag{46a}
\]

for any \( |\Delta w_1| < \delta_1 \). Next, from \((43)\) there exists an \( \delta_2 \) such that

\[
| \langle (\hat{y}' - \hat{y})^T, \nabla L(\hat{y}) \rangle | \geq |v_1 \Delta w_1 a| - |o(\Delta w_1)| b| \tag{47a}
\]

\[
> \frac{1}{2}|v_1 \Delta w_1 a| \tag{47b}
\]

and

\[
\text{sign} \left( \langle (\hat{y}' - \hat{y})^T, \nabla L(\hat{y}) \rangle \right) = \text{sign} \left( v_1 \Delta w_1 a \right) \tag{48}
\]
for any $|\Delta w_1| < \delta_2$.

By Lemma 5, there exists $\delta_3 > 0$ such that for any $\hat{y}' \in B_\delta(\hat{y}, \delta_3)$, if

$$\langle (\hat{y}' - \hat{y})^T, -\nabla L(\hat{y}) \rangle > \frac{|a|}{4||\partial z_1||_2} ||\hat{y}' - \hat{y}||_2$$

then $L(\hat{y}') < L(\hat{y})$.

Now we let $\Delta w_1 = -\lambda \text{sign}(v_1 a)$ where

$$0 < \lambda < \min \left\{ \epsilon, \delta_1, \delta_2, \frac{\delta_3}{2|v_1| \cdot ||\partial z_1||_2} \right\}.$$  (50)

First, we have $||w' - w||_2 = |\Delta w_1| = \lambda < \epsilon$, so the perturbation is within $B_\epsilon(\theta, \epsilon)$. Second, as $|\Delta w_1| < \delta_1$, (46) holds, yielding

$$||\hat{y}' - \hat{y}||_2 < 2|v_1 \Delta w_1| \cdot ||\partial z_1||_2$$

$$= 2\lambda |v_1| \cdot ||\partial z_1||_2$$

$$< \delta_3.$$  (51c)

Third, as $|\Delta w_1| < \delta_2$, (47a) and (48) hold, yielding

$$\langle (\hat{y}' - \hat{y})^T, -\nabla L(\hat{y}) \rangle = \lambda |v_1 a| + o(\Delta w_1)$$

$$> \frac{\lambda}{2} |v_1 a|$$

$$> \frac{|a|}{4||\partial z_1||_2} ||\hat{y}' - \hat{y}||_2$$

where (52c) follows from (51b). Combining (51) and (52), we have $L(\hat{y}') < L(\hat{y})$.

We complete the proof.

### C Proof of Theorem 2

From Assumption 3, $\sigma$ is linear in $(a - \delta, a + \delta)$, say

$$\sigma(t) = \alpha t + \beta, \ t \in (a - \delta, a + \delta).$$  (53)

Now we construct the weights to each hidden layer such that the following two conditions are satisfied.

1. $z_{h,i,n} \in (a - \delta, a + \delta), \forall i, n$;
2. row $(T_h(W)) = \text{row} \left( \begin{bmatrix} X^T \\ 1^T_N \end{bmatrix} \right)$.

Consider the weights to the first hidden layer. Notice that $d_1 > d_0$, we let

$$W_1 = V_1 \in \mathbb{R}^{d_1 \times d_0}$$  (54)
where \( V_1 \in \mathbb{R}^{d_1 \times d_0} \) satisfies \( \| V_1 X \|_F^2 < \delta/2 \), to be determined later. Let \( b_1 = a 1_{d_1} + u_1 \), where \( u_1 \in \mathbb{R}^{d_1} \) satisfies \( \| u_1 \|_2^2 < \delta/2 \), also to be determined later. Then we can verify that condition (1) holds for the first hidden layer. We further have

\[
T_1 = \sigma (W_1, b_1) \left[ X \begin{array}{c} 1_N \end{array} \right] \\
= a W_1 X + \alpha b_1 1_N + \beta 1_{d_1} \\
= a V_1 X + (ao + \beta) 1_{d_1} 1_N \\
= [\alpha V_1, \alpha u_1 + (ao + \beta) 1_{d_1}] X 1_N
\]

(55)

There exist \( V_1 \) and \( u_1 \) with

\[
\| V_1 X \|_F, \| u_1 \|_2 < \delta/2,
\]

such that row(\( T_1 \)) = row \( \left[ X \begin{array}{c} 1_N \end{array} \right] \).

(56)

Thus, condition (2) is also satisfied. If conditions (1) and (2) hold for the \((h-1)\)-th hidden layer, following a similar analysis, we can construct \( W_h \) and \( b_h \) to meet conditions (1) and (2) for the \(h\)-th hidden layer. As such, we construct \( W_{[1:H]} \). Finally, we consider the weights in the output layer, i.e., \( W_{H+1} \). We let

\[
W_{H+1} = \arg \min_{V \in \mathbb{R}^{d_{H+1} \times d_H}} \| Y - V T_H \|_F^2.
\]

(57)

which is a minimizer of a convex optimization problem. Note that condition (2) holds for the last hidden layer, and therefore \( W \) equivalently minimizes the distance from \( Y \) to row \( \left[ X \begin{array}{c} 1_N \end{array} \right] \), i.e.,

\[
E(W) = \min_{V \in \mathbb{R}^{d_{H+1} \times (d_H+1)}} \| Y - V \left[ X \begin{array}{c} 1_N \end{array} \right] \|_F^2.
\]

(58)

From Assumption 3, \( E(W) > 0 \).

To complete the proof, it suffices to show that the constructed \( W \) is indeed a local minimum. From Assumption 3 there exists \( \delta_1 \) such that for any \( W' \in B(W, \delta_1) \), the input of any hidden-layer neuron is within \((a - \delta, a + \delta)\). Then, it can be shown that for \( h = 1, 2, \cdots, H \),

\[
\text{row}(T_h(W')) \in \text{row} \left[ X \begin{array}{c} 1_N \end{array} \right].
\]

(59)

Therefore,

\[
E(W') = \| Y - W'_{H+1} T_H \left( W'_{[1:H]} \right) \|_F^2 \\
\geq \min_{V \in \mathbb{R}^{d_{H+1} \times (d_H+1)}} \| Y - V \left[ X \begin{array}{c} 1_N \end{array} \right] \|_F^2 \\
= E(W)
\]

(60)

Thus, \( W \) is a local minimum with \( E(W) > 0 \).

27
D Proof of Lemma 3

Without loss of generality, we assume \( [\sigma'(a)]^{H-1} \sigma''(a) > 0 \).

We first construct an \( N \times d_0 \) matrix \( X^{(1)} \) whose columns consist of all vectors in
\[
X_1 = \{ X_{(i,:)} \circ X_{(i,:)} \mid i = 1, 2, \ldots, d_0 \}
\]  
which is a subset of \( \mathcal{X} \), and an \( N \times (d_0^2 + 1) \) matrix \( X^{(2)} \) whose columns consist of all vectors in \( \mathcal{X} \setminus X_1 \).

As the vectors in \( \mathcal{X} \) are linearly independent, \( X^{(1)} \) and \( X^{(2)} \) are both full column rank, i.e., \( \text{rank}(X^{(1)}) = d_0 \) and \( \text{rank}(X^{(2)}) = d_0^2 + 1 \). Further, we have
\[
\text{rank} \left( \begin{bmatrix} X^{(1)} \\ X^{(2)} \end{bmatrix} \right) = d_0^2 + d_0 + 1.
\]  
This implies that there exists \( V \in \mathbb{R}^{d_0 \times N} \) such that
\[
V X^{(1)} = I, \quad V X^{(2)} = 0.
\]  
Now we construct each row of \( Y \) as
\[
Y_{(i,:)} = \hat{Y}_{(i,:)}(W) - \sum_{j=1}^{d_0} \alpha_{i,j} V_{(j,:)}, \quad i = 1, 2, \ldots, d_{H+1}
\]  
where each \( \alpha_{i,j} \) is an arbitrary positive value. Then, from (63) we have
\[
[\sigma'(a)]^{H-1} \sigma''(a) \cdot \langle \Delta Y_{(i,:)}(W), u_1 \rangle
\]  
for any \( u_1 \in X_1 \). Thus, (24d) is met. We also have
\[
\langle \Delta Y_{(i,:)}(W), u_2 \rangle = \sum_{j=1}^{d_0} \alpha_{i,j} \langle V_{(j,:)}(W), u_2 \rangle = 0
\]  
for any \( u_1 \in X_2 \). Thus, (24a)-(24c) are met. We complete the proof.

E Proof of Lemma 4

First, we show that for each hidden layer, we have the following claim.

Claim 1: For the \( h \)-th hidden layer, \( h = 1, 2, \ldots, H \), there exists \( \delta'_{h,i} \) such that for any \( W' \in B(W, \delta'_{h,i}) \) with \( W'_1 \neq W_1 \),
\[
[\sigma'(a)]^{(H-h)} \cdot \langle \Delta Y_{(i,:)}(W), (T_h)_{(j,:)}(W') - (T_h)_{(j,:)}(\hat{W}') \rangle > 0
\]
for \( i = 1, 2, \cdots, d_{H+1}, j = 1, 2, \cdots, d_h \).

We prove Claim 1 by induction. Noting that \( W_1 = 0 \), for the first hidden layer, we have

\[
(T_1)_{(i,:)}^T (W') - (T_1)_{(i,:)}^T (\tilde{W}') = \sigma \left((W_2')_{(i,:)}^T X + b'_{1,i,j}^T \right) - \sigma(b'_{1,i,j})^T \tag{68a}
\]

\[
= \sigma'(b'_{1,i,j})(W_1')_{(i,:)}^T X + \sigma''(b'_{1,i,j}) \cdot [(W_1')_{(i,:)}^T X] \circ [(W_1')_{(i,:)}^T X]
\]

\[
+ \mathbf{o}^T \left( \| (W_1')_{(i,:)}^T \|_2^2 \right) \tag{68b}
\]

\[
= \sigma'(b'_{1,i,j}) \left[(W_1')_{(i,:)}^T X\right] + \sigma''(b'_{1,i,j}) \left( \sum_{k=1}^{d_0} w'_{1,i,k} X_{(k,:)} \right) \circ \left( \sum_{k=1}^{d_0} w'_{1,i,k} X_{(k,:)} \right)^T
\]

\[
+ \mathbf{o}^T \left( \| (W_1')_{(i,:)}^T \|_2^2 \right) \tag{68c}
\]

where \( 68a \) follows from \( W_1 = 0 \), and \( 68b \) is obtained by performing Taylor expansion at \((Z_1)_{(i,:)}^T (\tilde{W}')\). From \( 24c \), we have

\[
\left< \Delta Y_{(i,:)}, \left[ \sigma'(b'_{1,i,j}) \cdot (W_1')_{(i,:)}^T X \right]^T \right> = \sigma'(b'_{1,i,j}) \sum_{k=1}^{d_0} w'_{1,i,k} \left< \Delta Y_{(i,:)}, X_{(k,:)} \right> = 0 \tag{69a}
\]

and from \( 24c \), we have

\[
\left< \Delta Y_{(i,:)}, \sigma''(b'_{1,i,j}) \left[ \sum_{k=1}^{d_0} w'_{1,i,k} X_{(k,:)} \right] \circ \left[ \sum_{k=1}^{d_0} w'_{1,i,k} X_{(k,:)} \right] \right>
\]

\[
= \sigma''(b'_{1,i,j}) \sum_{k=1}^{d_0} \left( w'_{1,i,k} \right)^2 \left< \Delta Y_{(i,:)}, X_{(k,:)} \circ X_{(k,:)} \right>
\]

\[
+ 2 \sigma''(b'_{1,i,j}) \sum_{k=1}^{d_0} \sum_{k'=1}^{d_0} w'_{1,i,k} w'_{1,i,k'} \left< \Delta Y_{(i,:)}, X_{(k,:)} \circ X_{(k',:)} \right>
\]

\[
= \sigma''(b'_{1,i,j}) \sum_{k=1}^{d_0} \left( w'_{1,i,k} \right)^2 \left< \Delta Y_{(i,:)}, X_{(k,:)} \circ X_{(k,:)} \right>. \tag{69b}
\]

With \( 68 \) and \( 69 \), we have

\[
\left< \Delta Y_{(i,:)}, (T_1)_{(i,:)}^T (W') - (T_1)_{(i,:)}^T (\tilde{W}') \right> = \sigma''(b'_{1,i,j}) \sum_{k=1}^{d_0} \left( w'_{1,i,k} \right)^2 \left< \Delta Y_{(i,:)}, X_{(k,:)} \circ X_{(k,:)} \right>
\]

\[
+ \left< \Delta Y_{(i,:)} \circ (W_1')_{(i,:)}^T \right> \tag{70}
\]
From [24d], each of the inner products $\langle \Delta Y_{(i,:)} X_{(k,:)} \rangle$ has the same sign with $[\sigma'(a)]^{H-1}\sigma''(a)$. Noting that $W'_1 \neq 0$, there exists at least one $w'_{1,j,k} \neq 0$. Then we have

$$\sigma''(a)[\sigma'(a)]^{H-1} \sum_{k=1}^{d_0} (w'_{1,j,k})^2 \langle \Delta Y_{(i,:)} X_{(k,:)} \rangle > 0 \quad (71)$$

Now, recall that we assume $W' \in B(W, \min\{\delta_1, \delta_2\})$, and hence [23] holds. There exists $\delta'_1 > 0$ such that for any $W' \in B(W, \delta'_1)$ with $W'_1 \neq W_1$, we have

$$|\sigma''(b'_{1,j})| > \frac{1}{2} |\sigma''(a)| \quad (72)$$

and

$$\left| \left\langle \Delta Y_{(i,:)}, o \left( \|W'_1\|_2^2 \right) \right\rangle \right| 
\leq \frac{1}{2} \sigma''(a) \sum_{k=1}^{d_0} (w'_{1,j,k})^2 \left| \langle \Delta Y_{(i,:)}, X_{(k,:)} \rangle \right| 
\leq \left| \sigma''(b'_{1,j}) \sum_{k=1}^{d_0} (w'_{1,j,k})^2 \left| \langle \Delta Y_{(i,:)}, X_{(k,:)} \rangle \right| \right| \quad (73)$$

Therefore,

$$\text{sign} \left( [\sigma'(a)]^{H-1} \langle \Delta Y_{(i,:)}, (T_h)_{(j,:)}(W') - (T_h)_{(j,:)}(\tilde{W}') \rangle \right) 
= \text{sign} \left( [\sigma'(a)]^{H-1} \sigma''(b'_{1,j}) \sum_{k=1}^{d_0} (w'_{1,j,k})^2 \left| \langle \Delta Y_{(i,:)}, X_{(k,:)} \rangle \right| \right) 
= \text{sign} \left( [\sigma'(a)]^{H-1} \sigma''(a) \sum_{k=1}^{d_0} (w'_{1,j,k})^2 \left| \langle \Delta Y_{(i,:)}, X_{(k,:)} \rangle \right| \right) 
= 1. \quad (74)$$

Claim 1 is valid for $h = 1$.

Now, consider an arbitrary $2 \leq h \leq H$, and suppose that Claim 1 holds for the $(h-1)$-th hidden layer.

$$\left( T_h \right)_{(j,:)}^T(W') - \left( T_h \right)_{(j,:)}^T(\tilde{W}') 
= \sigma \left( (W_h')_{(j,:)}^T T_{h-1}(W') - \sigma \left( (W_h')_{(j,:)}^T T_{h-1}(\tilde{W}') \right) \right) 
= \sigma' \left( (Z_{h-1})_{(j,:)}^T(\tilde{W}') \right) \circ \sigma' \left( (Z_{h-1})_{(j,:)}^T(\tilde{W}') \right) + o^T \left( \left\| (W_h')_{(j,:)} \left[ T_{h-1}(W') - T_{h-1}(\tilde{W}') \right] \right\|_2 \right) \quad (75)$$

From the induction hypothesis, $(T_h)_{(j,:)}(W') \neq (T_h)_{(j,:)}(\tilde{W}')$
Noting that each $w'_{h,j,k}$ is positive, there exists $\delta_{h,i}$ such that for any $W' \in B(W, \delta_{h,i})$ with $W_1' \neq W_1$, we have
\[
\sigma' \left( z_{h-1,j,n}(\tilde{W}') \right) \sigma(a)' > 0 \quad (76a)
\]
\[
|\sigma' \left( z_{h-1,j,n}(\tilde{W}') \right) | > \frac{1}{2} |\sigma'(a)| \quad (76b)
\]
for $n = 1, 2, \ldots, N$. Then
\[
\left| \left\langle \Delta Y_{(i,\cdot)}, \left\{ (W_h^T)_{(j,:)} \left[ T_{h-1}(W') - T_{h-1}(\tilde{W}') \right] \right\} \circ \sigma' \left( (Z_{h-1})_{(j,:)}(\tilde{W}') \right) \right\rangle \right|
\]
\[
> \frac{1}{2} \left| \left\langle \Delta Y_{(i,\cdot)}, \left\{ (W_h^T)_{(j,:)} \left[ T_{h-1}(W') - T_{h-1}(\tilde{W}') \right] \right\} \circ (\sigma'(a) \cdot 1) \right\rangle \right|
\]
\[
= \frac{1}{2} |\sigma'(a)| \cdot \sum_{k=1}^{d_{h-1}} |w_{h,j,k}'| \left| \left\langle \Delta Y_{(i,\cdot)}, (T_{h-1}(W') - (T_{h-1})(W')) \right\rangle \right|
\]
\[
> 0 \quad (77)
\]
Further, $\left\| T_{h-1}(W') - T_{h-1}(\tilde{W}') \right\|_2$ is sufficiently small such that
\[
\left| \left\langle \Delta Y_{(i,\cdot)}, \circ \left( \left\| (W_h^T)_{(j,:)} \left[ T_{h-1}(W') - T_{h-1}(\tilde{W}') \right] \right\|_2 \right) \right\rangle \right|
\]
\[
< \frac{1}{2} |\sigma'(a)| \cdot \sum_{k=1}^{d_{h-1}} |w_{h,j,k}'| \left| \left\langle \Delta Y_{(i,\cdot)}, (T_{h-1}(W') - (T_{h-1})(W')) \right\rangle \right|
\]
\[
< \left| \left\langle \Delta Y_{(i,\cdot)}, \left\{ (W_h^T)_{(j,:)} \left[ T_{h-1}(W') - T_{h-1}(\tilde{W}') \right] \right\} \circ \sigma' \left( (Z_{h-1})_{(j,:)}(\tilde{W}') \right) \right\rangle \right|. \quad (78)
\]
Therefore,
\[
\text{sign} \left( [\sigma'(a)]^{(H-h)} \cdot \left\langle \Delta Y_{(i,\cdot)}, (T_{h})(W') - (T_{h})(\tilde{W}') \right\rangle \right)
\]
\[
= \text{sign} \left( [\sigma'(a)]^{(H-h+1)} \sum_{k=1}^{d_{h-1}} w_{h,j,k}' \left\langle \Delta Y_{(i,\cdot)}, (T_{h-1})(W') - (T_{h-1})(\tilde{W}') \right\rangle \right)
\]
\[
= 1 \quad (79)
\]
We complete the proof of Claim 1.

For the output layer, we have the following claim. Note that based on Claim 1, Claim 2 can be shown in the same way with (76) and (79). We omit the detailed proof of Claim 2 here.

**Claim 2:** There exists $\delta_3 > 0$ such that for any $W' \in B(W, \delta_3)$ with $W_1' \neq W_1$,
\[
\left\langle \Delta Y, \hat{Y}(W') - \hat{Y}(\tilde{W}') \right\rangle_F > 0. \quad (80)
\]

At last, for any $W' \in B(W, \delta_3)$ with $W_1' = W_1$, we have $W' = \tilde{W}'$. Thus
\[
\left\langle \Delta Y, \hat{Y}(W') - \hat{Y}(\tilde{W}') \right\rangle_F = \left\langle \Delta Y, 0 \right\rangle_F = 0. \quad (81)
\]
Combining Claim 2, we complete the proof of Lemma.