Understanding Global Loss Landscape of One-hidden-layer ReLU Neural Networks

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Abstract
For one-hidden-layer ReLU networks, we show that all local minima are global in each differentiable region, and these local minima can be unique or continuous, depending on data, activation pattern of hidden neurons and network size. We give criteria to identify whether local minima lie inside their defining regions, and if so (we call them genuine differentiable local minima), their locations and loss values. Furthermore, we give necessary and sufficient conditions for the existence of saddle points as well as non-differentiable local minima. Finally, we compute the probability of getting stuck in genuine local minima for Gaussian input data and parallel weight vectors, and show that it is exponentially vanishing when the weights are located in regions where data are not too scarce. This may give a hint to the question why gradient-based local search methods usually do not get trapped in local minima when training deep ReLU neural networks.

1 Introduction
One of the greatest mysteries in deep learning is that despite the highly non-convex nature of loss functions, local search based optimization methods, such as gradient descent, still often succeed in practice. Understanding the global landscape of loss functions, especially whether bad local minima and saddle points exist, their count and locations if they do exist, will contribute greatly to solving this puzzle. Based on these understandings, it is possible to design search algorithms that are insensitive to initial weights and guaranteed to escape all bad local minima and saddle points effectively.

It has been shown that there are no bad local minima for some specific types of networks, including deep linear networks, one-hidden-layer networks with quadratic activation, very wide networks, and networks with special type of extra neurons (see subsection 1.1 for related works). In other words, all local minima are global for these networks and there is no chance of getting stuck in bad local minima. However, in general this is not true for ReLU networks which are widely used in practice, as evidenced in the studies of e.g., [Safran & Shamir (2018); Swirszcz et al. (2016); Zhou & Liang (2018); Yun et al. (2019)]. The weight space of ReLU networks is divided into differentiable regions and non-differentiable ones due to the non-smoothness introduced by ReLU activation. It is unclear in theory that for ReLU networks of any size and any input, existence of non-differentiable local minima requires what conditions, and how the probability of existing local minima varies in the weight space. On the other hand, in spite of works on escaping saddle points, an analytical exploration of saddle points for ReLU networks, including the conditions for their existences and their locations, is still missing to a large extent.

In this paper, we seek to understand the global loss landscape of one-hidden-layer ReLU networks, in the hope of giving inspirations to the understanding of general deep ReLU networks. More specifically, for one-hidden-layer ReLU networks of any size (not just over-parameterized case where network size is much bigger than the number of samples), we have made the following contributions in this paper.
• We show that in each differentiable region all local minima are global (i.e., there are no bad local minima in each differentiable region). We show that local minima can be unique or continuous, depending on data, activation pattern of hidden-layer neurons and network size. We find the locations of local minima for each differentiable region at first. Then, we give criteria to test whether they are really inside their defining regions.

• We give necessary and sufficient conditions for the existence of saddle points, as well as non-differentiable local minima which lie on the boundaries between differentiable regions, and their locations if they do exist.

• We compute the probability of existing genuine local minima for Gaussian input data and parallel weight vectors, and show that it is exponentially vanishing when the weights are not far away from data distribution peaks.

This paper is organized as follows. Section 1.1 is related work. Section 2 gives the preliminaries and describes the one-hidden-layer ReLU network model. In section 3, we show that all local minima are global for differentiable regions. Section 4 presents conditions for existence of genuine differentiable local minima and their locations, and illustrates the single point and continuous cases of local minima with a simple example. We give the necessary and sufficient conditions for saddle points in section 5, and for non-differentiable local minima in section 6. In section 7, we compute the probability of hitting local minima for Gaussian input, and demonstrate how this probability varies in weight space with experiments. Finally, we conclude this paper and point out future directions. The detailed proofs of our lemmas and theorems will be deferred to the Appendix.

1.1 Related work

Loss landscape Matrix completion and tensor decomposition, e.g., Ge et al. (2016) are learning models involving the product of two unknown matrices, and it has been shown that all local minima are global for such models. Deep linear networks, which remove the non-linear activation function of each neuron in multi-layer perceptions, also do not have spurious local minima according to Kawaguchi (2016); Lu & Kawaguchi (2017); Laurent & von Brecht (2018a); Yun et al. (2018); Nouiehed & Razaviyayn (2018); Zhang (2019); Hardt & Ma (2017) shows deep linear residual networks have no spurious local optima. Choromanska et al. (2015) uses spin glass models in statistical physics to analyze the landscape which simplifies the nonlinear nature of deep neural networks.

For one-hidden-layer over-parameterized networks with quadratic activation, Soltanolkotabi et al. (2019); Du & Lee (2018) prove that all local minima are global. For one-hidden-layer ReLU networks, Soudry & Carmon (2016) gives the conditions under which loss at differentiable local minima is zero, thus being global minima. [Laurent & von Brecht] (2018b) shows that ReLU networks with hinge loss can only have non-differentiable local minima and gives the conditions for their existence for linear separable data. Safran & Shamir (2016) shows that there is a high probability of initializing at a basin with small minimal loss for over-parameterized one-hidden-layer ReLU networks. Soudry & Hoffer (2017) exhibits that, given standard Gaussian input data, the volume of differentiable regions containing sub-optimal differentiable local minima is exponentially vanishing in comparison with that containing global minima.

Absence of spurious valley for ultra-width networks are explored in Venturi et al. (2018); Nguyen & Hein (2019); Li et al. (2018a); Nguyen et al. (2019); Ding et al. (2019); Liang et al. (2018b); Kawaguchi & Kaelbling (2019) show that by adding a single-layer network or even a single special neuron in the shortcut connection, every local minimum becomes global. Ge et al. (2017); Gao et al. (2018); Feizi et al. (2017) design new loss functions or special networks so that all local minima are global. Shamir (2018); Kawaguchi & Bengio (2018) prove that depth with nonlinearity creates no bad local minima in a type of ResNets in the sense that the values of all local minima are no worse than that of global minima of corresponding shallow linear predictors. Pennington & Worah (2018); Pennington & Bahri (2017) use random matrix theory to study the spectrum of Hessians of loss functions, which characterizes the landscape in the neighborhood of stationary points. Mei et al. (2016); Zhou & Feng (2018) study the landscape of expected loss.

Saddle points Dauphin et al. (2014) argue that a main source of difficulty for local search based optimization methods comes from the proliferation of saddle points. Yun et al. (2018) gives the conditions that distinguish saddle points from local minima for deep linear networks. Jin et al.
(2018b) adopts hinge loss and linear separable data, while our theory is general and

Empirical studies of landscape Besides theoretical researches, there have been some experimental
explorations on visualization of landscape [Goodfellow et al. (2015), Liao & Poggio (2017), Li et al.
(2018b), geometry of level sets [Freeman & Bruna (2017)] and mode connectivity [Draxler et al. (2018),
Garipov et al. (2018)].

Convergence of gradient based optimization There have been many works on the convergence of
gradient based methods for training deep neural networks. Some recent works, e.g., Du et al. (2019),
Allen-Zhu et al. (2019), Zou et al. (2018) show that gradient descent always converges for fully
connected, convolutional and residual networks if they are wide enough, the step-size is small enough
and the weights are Gaussian initialized. However, convergence analysis for networks of any size and
arbitrary initial weights still requires an understanding of global landscape.

Comparisons with our work The works most related to ours are Soudry & Carmon (2016), Laurent
& von Brecht (2018b), Safran & Shamir (2016), Soudry & Hoffer (2017), Safran & Shamir (2018),
Zhou & Liang (2018), of them dealing with local minima of one-hidden-layer ReLU networks. Comparing
with our work, Soudry & Carmon (2016) considers only over-parameterized case, Laurent
& von Brecht (2018b) adopts hinge loss and linear separable data, while our theory is general and
applies to one-hidden-layer ReLU networks of any size and any input. Safran & Shamir (2016)
computes the probability of getting trapped in the basin that contains global minima, whereas our
theory considers how the probability of existing genuine local minima varies in the whole weight
space. The experimental study of Safran & Shamir (2018) uses a student-teacher objective that is
different than ours. Soudry & Hoffer (2017) calculates the probability of having bad local minima.
However, their concept of bad local minima is different from ours in the sense that they refer to
local minima with nonzero loss, which may not be genuine ones for locating outside their defining
basins. Comparing with Zhou & Liang (2018), our proof of no spurious local minima in differentiable
regions is different and simpler, and we propose to identify genuine local minima using intersection
of hyperplanes.

2 One-hidden-layer ReLU neural network model and Preliminaries

In the one-hidden-layer ReLU network model studied in this paper, there are \( K \) hidden neurons
with ReLU activation, \( d \) input neurons and one output neuron. We use \( \{N\} \) to denote \( \{1, 2, \cdots, N\} \).
The input samples are \( (x_i, y_i) (i \in \{N\}) \), where \( x_i \in \mathbb{R}^d \) is the \( i \)th homogeneous data vector (i.e.,
augmented with scalar 1) and \( y_i \in \{-1, 1\} \) is the label of \( x_i \). We make no assumptions on the network size
and input data. Denoting the weight vectors connecting hidden neurons and input as \( (w_i, i \in \{K\}) \)
augmented with bias), and the weights between output neuron and hidden ones as \( (z_i, i \in \{K\}) \),
the loss of one-hidden-layer ReLU networks is

\[
L(z, w) = \frac{1}{N} \sum_{i=1}^{N} \left( \sum_{j=1}^{K} z_j \cdot (w_j \cdot x_i)_+ + y_i \right),
\]

where \( z = \{z_k, k \in \{K\}\}, w = \{w_k, k \in \{K\}\}, \) \( (y)_+ = \max(0, y) \) is the ReLU function, and \( l \) is
the loss function. We assume \( l \) is convex, which is true for the commonly used squared loss and
cross-entropy loss.

Moore-Penrose inverse of matrices [Horn & Johnson (2012)] will be heavily used in this paper. \( M^+ \)
denotes the Moore-Penrose inverse of a matrix \( M \in \mathbb{R}^{m \times n} \). It satisfies the following four equations:

\[
MM^+ M = M, M^+ MM^+ = M^+, (MM^+)^T = MM^+, (M^+ M)^T = M^+ M.
\]

Therefore, \( MM^+ \) is symmetric, and \( M^+ = I_m \) if and only if \( \text{rank}(M) = m \) and \( M^+ M = I_n \)
if and only if \( \text{rank}(M) = n \), where \( I_m \) is the \( m \times m \) identity matrix. If \( M \in \mathbb{R}^{m \times m} \) \( (r > 0) \) is
the rank of \( M \), and the full-rank decomposition of \( M = FG \) \( (F \in \mathbb{R}^{r \times m}, G \in \mathbb{R}^{m \times r}) \),
then \( M^+ = G^T (GG^T)^{-1} (F^T)^{-1} F^T \). For \( b \in \mathbb{R}^m \), the general solution to the least square problem
\( \min_x \|Mz - b\|_2^2 \) is \( z = M^+ b + (I - M^+ M) c, (c \in \mathbb{R}^n \) is arbitrary). The necessary and sufficient
conditions for the linear system \( Mz = b \) to be solvable are \( MM^+ b = b \), and the general solution is
also \( z = M^+ b + (I - M^+ M) c \).
3 All differentiable local minima are global

Let us rewrite the loss into a form that will simplify our problems. Introducing variables \( I_{ij} \) which equal 1 if \( w_j \cdot x_i > 0 \) and 0 otherwise, the loss can be rewritten as

\[
L(z, w) = \frac{1}{N} \sum_{i=1}^{N} \left( \sum_{j=1}^{K} z_j \cdot I_{ij} w_j \cdot x_i, y_i \right).
\]

Defining \( R_j = z_j w_j \), which integrates the weights of two layers, the loss is converted into

\[
L(R) = \frac{1}{N} \sum_{i=1}^{N} \left( \sum_{j=1}^{K} I_{ij} R_j \cdot x_i, y_i \right),
\]

where \( R = \{ R_k, k \in [K] \} \). This conversion is key to our proofs in subsequent sections. It hides the complexity of having two layer weights to a large degree.

For one-hidden-layer ReLU network model, \( x \) is a hyperplane in the space of \( w \), and the samples \( (x_i, i \in [N]) \) partition the \( w \) space into a number of convex cells, such as cell 1 and cell 2 shown in fig.1. Each weight \( w_j \) is therefore located in a certain cell or on the boundary of cells. If all weights \( (w_j, j \in [K]) \) are located inside cells and move within them without crossing the boundaries, \( I_{ij} \) will have constant values, and thus loss \( L \) is a differentiable function of \( (R_j, j \in [K]) \) within these cells. We call the cells inside which \( (w_j, j \in [K]) \) reside as their defining cells. When crossing the boundary of two cells, such as from cell 2 and to cell 1 in fig.1, \( I_{21} \) will change from 1 to 0 at the boundary. Therefore, loss \( L \) is non-differentiable at the boundaries. Local minima may exist inside cells or on the boundaries, and we call them differentiable and non-differentiable local minima respectively.

![Figure 1: Samples partition the weight space into cells.](image)

The detailed proof is given in Appendix A, here we present the proof sketch. At any differentiable local minimum \( (\hat{z}, \hat{w}) \), the derivatives \( \frac{\partial L}{\partial z_j} (\hat{z}, \hat{w}) \) exist and are all equal to 0. By \( R_j = z_j w_j \), we have

\[
\frac{\partial L}{\partial z_j} (\hat{z}, \hat{w}) = \frac{\partial L}{\partial R_j} (\hat{R}_1, \ldots, \hat{R}_K) \cdot \hat{w}_j = 0,
\]

\[
\frac{\partial L}{\partial w_j} (\hat{z}, \hat{w}) = \frac{\partial L}{\partial R_j} (\hat{R}_1, \ldots, \hat{R}_K) \cdot \hat{z}_j = 0, \quad (j \in [K]),
\]

where \( \hat{R}_j = \hat{z}_j \hat{w}_j \). If \( \hat{z}_j \neq 0 \), (4) implies \( \frac{\partial L}{\partial R_j} = 0 \), and (3) will be satisfied automatically. If \( \hat{z}_j = 0 \), (4) is satisfied, we only need to prove \( \frac{\partial L}{\partial R_j} = 0 \) from (3) for the case \( \hat{z}_j = 0 \).

The following Theorem 1 establishes the globalness of differentiable local minima, whose proof is given in Appendix A.
Theorem 1. If loss function $l$ is convex, then any differentiable local minimum of $L(z, w)$ is a global minimum. Furthermore, there are no local maxima for $L(z, w)$.

Although differentiable local minima are global in their defining regions, they are usually still local minima in the global landscape. In addition, despite $L(R)$ has a unique global minimum (unless some $R_j$ are not involved in $L$, see subsection 4.1), $(z, w)$ that achieves global minimal loss is not unique. Due to $R_j = z_j w_j = c z_j \cdot \hat{z} w_j$ when $c \neq 0$, as a result, if $\{c z_j, \hat{z} w_j\}$ achieves global minimal loss, so does $\{c z_j, \hat{z} w_j\}$.

4 Criteria for Existence of Differentiable Local Minima and Their Locations

Theorem 1 states that in each cell, all local minima of $L(z, w)$ are global. In this section, we first find out the locations of $\{z_j^*, w_j^*; j \in [K]\}$ that achieve global minima, then give the criteria to judge whether $\{w_j^*; j \in [K]\}$ are inside the defining cells and consequently being genuine differentiable local minima.

4.1 The Locations of Differentiable Local Minima

From now on, in order to get analytical solutions we assume that loss function $l$ is the squared loss. Lemma 1 implies that for differentiable local minima, there are $\partial L/\partial R_j = 0 (j \in [K])$, which actually amounts to solving the following least-square problem,

$$R^* = \arg \min_R \frac{1}{N} \sum_{i=1}^{N} \left( \sum_{j=1}^{K} I_{ij} R_j \cdot x_i - y_i \right)^2. \quad (5)$$

The associated linear system $\sum_{j=1}^{K} I_{ij} R_j \cdot x_i = y_i (i \in [N])$ can be rewritten in the following form

$$AR = y, A = \begin{pmatrix} I_{11} x_1^T & \cdots & I_{1K} x_1^T \\ \vdots & \ddots & \vdots \\ I_{N1} x_N^T & \cdots & I_{NK} x_N^T \end{pmatrix}, y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}, \quad (6)$$

where $R = (R_1^T \ldots R_K^T)^T$. Here we have changed the meaning of $R$ from a set in $\mathbb{R}$ to a vector without hampering the understanding. According to matrix theory, for the non-square matrix $A \in \mathbb{R}^{N \times Kd}$, the general solution $R^*$ to the least square problem $\mathbb{5}$ can be expressed as follows using Moore-Penrose inverse of $A$,

$$R^* = A^+ y + (I - A^+ A) c, \quad (7)$$

where $c \in \mathbb{R}^{Kd}$ is an arbitrary vector, $I$ is the identity matrix.

The optimal solution $R^*$ can be characterized by the following cases:

1). $R^*$ is unique: $R^* = A^+ y$, corresponding to $A^+ A = I$ and thus $(I - A^+ A) c$ vanishes. This happens if and only if $\text{rank}(A) = K d$. Therefore, $N \geq K d$ is necessary in order to have a unique solution. Using the full-rank decomposition when $A$ has full rank: $A^+ = (A^T A)^{-1} A^T$, the solution can be written as

$$R^* = (A^T A)^{-1} A^T y. \quad (8)$$

$\mathbb{8}$ can also be obtained by solving the linear system resulted from $\partial L/\partial R_j = 0 (j \in [K])$, an approach we will take for saddle points etc. later in this paper.

2). $R^*$ has infinite number of continuous solutions. In this case, $I - A^+ A \neq 0$, hence the arbitrary vector $c$ plays a role. This happens only when $\text{rank}(A) \neq K d$. As a result, there are two possible situations in which infinite number of optimal solutions exist. a). $N < K d$. This is usually referred to as over-parameterization and $AR = y$ has infinite number of solutions, with some components of $R$ being free variables. b). $N \geq K d$ but $\text{rank}(A) \neq K d$. One example is that some hidden units are not activated by all samples (i.e., $I_{ij} = 0$ for $i \in [N]$. The corresponding columns in $A$ are zeros).
Figure 2: An illustrative example of loss landscape with two samples. (a) $y_1 = 1$, $y_2 = 1$. (b) $y_1 = 1$, $y_2 = -1$.

$\mathbf{R}_j$ associated with such hidden neurons do not affect loss $L$, hence can be changed freely. A special occasion is that all hidden units are not activated by any sample, leading to $A = 0$ and consequently $A^+ = 0$ and $\mathbf{R}^* = \mathbf{c}$. In this case, $\mathbf{R}^*$ can be any vector in the whole weight space.

In general, (7) shows $\mathbf{R}^*$ is a affine transformation of $\mathbf{c} \in \mathbb{R}^{Kd}$. Therefore, $\mathbf{R}^*_j$ could be the whole $\mathbb{R}^d$ space or a linear subspace of it, depending on whether the rows in $(I - A^+ A)$ corresponding to $\mathbf{R}^*_j$ is of full rank or not.

To get the loss at these minima, we substitute (7) into the loss $L = \frac{1}{N} \| \mathbf{A} \mathbf{R}^* - \mathbf{y} \|_2^2$ and get

$$L(\mathbf{R}^*) = \frac{1}{N} \| \mathbf{A} A^+ \mathbf{y} - \mathbf{y} \|_2^2$$

The loss $L$ will be 0 only when $\mathbf{A} A^+ \mathbf{y} = \mathbf{y}$, corresponding to that the original linear system $\mathbf{A} \mathbf{R} = \mathbf{y}$ has solutions.

### 4.2 An Illustrative Example

We give a very simple example to illustrate different cases of differential local minima. Suppose there is only one hidden neuron, and there are two samples in the two-dimensional input space: $\mathbf{x}_1 = (1 \ 0)^T$, $\mathbf{x}_2 = (0 \ 1)^T$ with labels $y_1 = 1$, $y_2 = 1$. We set $z = 1$ and bias $b = 0$. The two samples become two vectors in the space of $\mathbf{w}$ and hence there are in total four cells. We can compute the locations and loss values of local minima in each cell using (7) and (9), and the details are presented in Appendix B. Fig. 2(a) shows the whole landscape, from which one can see that there are no spurious differential local minima in each cell, and the differential local minima are either a single point, a line or a flat plateau.

### 4.3 Criteria for Existence of Genuine Differentiable Local Minima

In the above example, if $y_2 = -1$, $\mathbf{R}^*$ for cell $r_4$ (the upper right one) will be $(1 \ -1)^T$, which is actually outside $r_4$. In this situation, the landscape of $r_4$ has no differential local minima at all, as shown in Fig. 2(b). In this subsection, we are going to present conditions under which $\mathbf{R}^*$ will be inside their defining cells. In line with different cases of $\mathbf{R}^*$, the criteria for each case are discussed as follows.

1. For the case $\mathbf{R}^*$ is unique, in order for $\mathbf{w}^*$ to be inside the defining cells, $\mathbf{w}^*$ should be on the same side of each sample with any point in these cells. Giving $I_{ij}$ ($i \in [N]; j \in [K]$) that specify the defining cells, this can be expressed as

$$\mathbf{w}^*_j \cdot \mathbf{x}_i \begin{cases} > 0 & \text{if } I_{ij} = 1; \\ \leq 0 & \text{if } I_{ij} = 0; \end{cases} (i \in [N]; j \in [K]).$$

Since $\mathbf{R}^*_j = z^*_j \mathbf{w}^*_j$, the conditions transform into $\frac{1}{z^*_j} \mathbf{R}^*_j \cdot \mathbf{x}_i \geq 0$. Except for its sign, the magnitude of $z^*_j$ does not affect the conditions, and consequently for given $\mathbf{R}^*_j$ the differentiable local minima $(z^*_j, \mathbf{w}^*_j)$ have two branches, corresponding to different signs of $z^*_j$. As a result, the criteria for existence of unique differentiable local minima can be expressed as: for each $\mathbf{R}^*_j$ ($j \in [K]$),

$$\mathbf{R}^*_j \cdot \mathbf{x}_i \begin{cases} > 0 & \text{if } I_{ij} = 1; \\ \leq 0 & \text{if } I_{ij} = 0; \end{cases} (i \in [N]).$$
or \( \mathbf{R}_j^* \cdot \mathbf{x}_i \begin{cases} < 0 & \text{if } I_{ij} = 1; \\ \geq 0 & \text{if } I_{ij} = 0; \\ \end{cases} (i \in [N]) \) (12)

2. For the case \( \mathbb{R}^n \) is continuous, we need to test whether the continuous differentiable local minima in (7) are in their defining cells. For example, substituting (7) into (11), then for each \( \mathbf{R}_j^* (j \in [K]) \) the criteria become

\[
x^T_j ((A^+ \mathbf{y})_j + (I - A^+) \mathbf{y}) \begin{cases} > 0 & \text{if } I_{ij} = 1; \\ \leq 0 & \text{if } I_{ij} = 0; \\ \end{cases} (i \in [N]) \tag{13}
\]

where \((A^+ \mathbf{y})_j\) is the rows of \(A^+ \mathbf{y}\) corresponding to \(\mathbf{R}_j^*\), and so on. Each inequality of \(c\) in (13) defines a half-space in \(\mathbb{R}^{K \times d}\). Therefore, the criteria for existing genuine continuous differentiable local minima reduce to identifying whether the intersection of all these half-spaces is null. The non-null intersection will be a convex high-dimensional polyhedron.

Another way to judging the existence of genuine continuous differentiable local minima is to extract \(\mathbf{R}_j^*\) from (7) at first, which is either the whole \(\mathbb{R}^d\) space or a linear subspace of it depending on whether the rows in \((I - A^+) \mathbf{y}\) is of full rank or not. If all \(\mathbf{R}_j^* (j \in [K])\) are the whole \(\mathbb{R}^d\) space, then any point in the defining cells is a genuine differentiable local minima. One example is the flat plateau region in fig. 2. If \(\mathbf{R}_j^*\) is a linear subspace of \(\mathbb{R}^d\), we can compute the cells in advance (apply arrangement algorithms [de Berg et al., 2008] to hyperplanes of samples) and then for each \(\mathbf{R}_j^* (j \in [K])\), find the intersection of its defining cell and linear subspace. If all intersections are not null, there exist continuous genuine differentiable local minima.

5 Saddle Points

5.1 Necessary and Sufficient Conditions for Existence of Differentiable Saddle Points

Unlike local minima, saddle points are stationary points that have both ascent and descent directions in their neighborhood, and thus their Hessians are indefinite.

Since saddle points are stationary points, (3) and (4) still hold. Form (4), \(z_j = 0\) if \(\frac{\partial L}{\partial w_j} \neq 0\). On the other hand, if \(\frac{\partial L}{\partial w_j} = 0\), (3) and (4) are both satisfied. However, \(\frac{\partial L}{\partial w_j} (j \in [K])\) can not all equal zero, otherwise the solutions would be differentiable local minima rather than saddle points. We need to test all possible combinations of the form \((j_1, j_2, \cdots, j_{K'}; K' < K)\) such that \(\frac{\partial L}{\partial w_j} = 0 (j = j_1, j_2, \cdots, j_{K'})\) and the remaining \(\frac{\partial L}{\partial w_j} (j = j_{K'+1}, \cdots, j_K)\) are non-zero, where \((j_1, j_2, \cdots, j_{K'})\) is any permutation of \((1, 2, \cdots, K)\), and see whether there exist saddle points.

The conditions for existence of differentiable saddle points are given in the following theorem.

**Theorem 2.** For the loss in (1) with \(l\) being the squared loss, there exist differentiable saddle points for all combinations of the form \((j_1, j_2, \cdots, j_{K'}; K' < K)\), where \((j_1, j_2, \cdots, j_{K'})\) is any permutation of \((1, 2, \cdots, K)\), and optimal \(\{\mathbf{R}_j^* (j = j_1, j_2, \cdots, j_{K'})\}\) of saddle points are the solutions to the linear system \(\mathbf{BR} = \mathbf{b}\), where \(\mathbf{R} = (\mathbf{R}_{j_1}^T, \mathbf{R}_{j_2}^T, \cdots, \mathbf{R}_{j_{K'}}^T)^T\), \(\mathbf{B} \in \mathbb{R}^{K' \times K' \times d}\) is a block matrix and \(\mathbf{b} \in \mathbb{R}^{K' \times d}\) is a block vector with the following components,

\[
B(j, k) = \sum_{i=1}^{N} I_{ij} \mathbf{x}_i \cdot I_{ik} \mathbf{x}_i^T,
\]

\[
b(j) = \sum_{i=1}^{N} I_{ij} \cdot y_i \mathbf{x}_i, \quad (j, k = j_1, j_2, \cdots, j_{K'}). \tag{14}
\]

**Optimal** \(\{\mathbf{R}_j^* (j = j_{K'+1}, \cdots, j_K)\}\) of saddle points satisfy

\[
\sum_{i=1}^{N} e_i I_{ij} \mathbf{x}_i \cdot \mathbf{w}_j^* = 0, \tag{15}
\]

where the error \(e_i = \sum_{k=j_1}^{j_{K'}} I_{ik} \mathbf{R}_k^* \cdot \mathbf{x}_i - y_i\).
As in subsection 4.1, $\boldsymbol{R}_j^* (j = j_1, j_2, \cdots, j_{K_f})$ may be unique or continuous. On the other hand, \textbf{[15]} indicates $\boldsymbol{w}_j^* (j = j_{K_f+1}, \cdots, j_K)$ is on a hyperplane that passes the origin in the space of $\boldsymbol{w}_j$. The proof of Theorem 2 will be presented in Appendix C.1.

Solutions provided in Theorem 2 may be not genuine differentiable saddle points. Conditions for their existence will be discussed in Appendix C.2.

6 Non-differentiable Local Minima

We consider the case that a weight vector lies on the boundary of two cells and thus the loss function $L$ in \textbf{[4]} is non-differentiable. Suppose $\boldsymbol{w}_m$ is located on the boundary of cell 1 and cell 2, separated by a sample $\mathbf{x}_n$. We are going to give the necessary and sufficient conditions for \{ $z_j (j \in [K])$: $\boldsymbol{w}_j$ is non-differentiable minimum if and only if $\partial L / \partial \mathbf{w}_m$ is non-differentiable. In the following lemma, we give the constraints $\partial L / \partial \mathbf{w}_m$ should satisfy in order for $\mathbf{w}_m$ to be a local minimum.

Lemma 2. Suppose $\overline{\mathbf{w}}_m$ lies on the boundary of cell 1 and cell 2 separated by sample $\mathbf{x}_n$, where cell 2 is on the positive side of $\mathbf{x}_n$ and cell 1 on negative side. $\overline{\mathbf{w}}_m$ is a non-differentiable minimum if and only if

$$\lim_{\mathbf{w}_m \to \overline{\mathbf{w}}_m} \frac{\partial L}{\partial \mathbf{w}_m} \mid_{1} / / (-\mathbf{x}_n), \lim_{\mathbf{w}_m \to \overline{\mathbf{w}}_m} \frac{\partial L}{\partial \mathbf{w}_m} \mid_{2} / / (\mathbf{x}_n)$$

where $\mathbf{a} / / \mathbf{b}$ denotes vectors $\mathbf{a}$ and $\mathbf{b}$ are in the same directions, $\partial L / \partial \mathbf{w}_m \mid 1$ means $\partial L / \partial \mathbf{w}_m$ in cell 1.

The conditions for existence of non-differentiable local minima are given by the following theorem.

Theorem 3. For the loss in \textbf{[1]} with $l$ being the squared loss, there exist non-differentiable local minima that reside on the boundary of two cells if and only if the linear system $\mathbf{D} \mathbf{R} = \mathbf{d}$ has solutions for any $m \in [K]$, where $\mathbf{D} \in \mathbb{R}^{(K+1)d \times K \cdot d}$ is a matrix and $\mathbf{d} \in \mathbb{R}^{(K+1)d}$ is a vector with the following block components,

$$D(j, k) = \sum_i I_{ij} I_{ik} \mathbf{x}_i \mathbf{x}_i^T \quad (j, k \in [K], j \neq m),$$

$$D(m, k) = \sum_{i \neq n} I_{im} I_{ik} (\mathbf{x}_i \cdot \mathbf{x}_n - |\mathbf{x}_n|^2 \mathbf{x}_i) \mathbf{x}_i^T \quad (k \in [K]),$$

$$D(K + 1, m) = \mathbf{x}_n^T, \quad D(K + 1, k) = 0 \quad (k \in [K], k \neq m),$$

$$\mathbf{d}(j) = \sum_i I_{ij} y_i \mathbf{x}_i \quad (j \in [K], j \neq m), \quad \mathbf{d}(K + 1) = 0,$$

$$\mathbf{d}(m) = \sum_{i \neq n} I_{im} y_i (\mathbf{x}_i \cdot \mathbf{x}_n - |\mathbf{x}_n|^2 \mathbf{x}_i), \quad (17)$$

and its solution $\mathbf{R}^*$ satisfies the following two inequalities for either $z_m > 0$ or $z_m < 0$,

$$\sum_{i \neq n} \left[ \sum_k (I_{ik} \mathbf{R}_k^* \cdot \mathbf{x}_i - y_i) I_{im} \mathbf{x}_i \cdot \mathbf{x}_n \right] z_m < 0, \quad (18)$$

$$\sum_{i \neq n} \left[ \sum_k (I_{ik} \mathbf{R}_k^* \cdot \mathbf{x}_i - y_i) I_{im} \mathbf{x}_i \cdot \mathbf{x}_n \right] z_m + \sum_k (I_{nk} \mathbf{R}_k^* \cdot \mathbf{x}_n - y_n) |\mathbf{x}_n|^2 z_m > 0. \quad (19)$$

The linear system in Theorem 3 has solutions if and only if $\mathbf{D}^+ \mathbf{d} = \mathbf{d}$. If solvable, its general solution is $\mathbf{R}^* = \mathbf{D}^+ \mathbf{d} + (I - \mathbf{D}^+ \mathbf{D}) \mathbf{c}$. If $\mathbf{R}^*$ is not unique, each inequality in \textbf{(18)} and \textbf{(19)} will confine $\mathbf{c}$ in a half-space. Therefore, there exist non-differentiable local minima if the intersection of these half-spaces is not null. The proofs of Lemma 2 and Theorem 3 will be given in Appendix D.1, and conditions for existence of genuine non-differentiable local minima in Appendix D.2.
7 Probability of Existing Genuine Local Minima

7.1 Locations of Local Minima when All Weight Vectors are Parallel

In this section, we will compute the probability of existing genuine local minima for Gaussian input data, and show how this probability changes with network weights. The core idea is that if no samples lie between the original weight vector \( \mathbf{w} \) and the local minima \( \mathbf{w}^* \), then (10) will hold and \( \mathbf{w}^* \) will be inside the same cell with \( \mathbf{w} \), hence a genuine local minima. Therefore, the probability of existing genuine local minima is actually the probability of having no samples between \( \mathbf{w} \) and \( \mathbf{w}^* \). However, it is complex to get an analytical probability starting from the general solution of \( \mathbf{w}^* \) in (8). Instead, we will impose some restrictions to simplify the solutions.

More specifically, we suppose all weights are parallel. Using unit vector \( \mathbf{i} \) to denote the directions of weight vectors, a weight \( \mathbf{w}_k \) is represented by its normal \( \mathbf{n}_k = \mathbf{i} \) or \( \mathbf{n}_k = -\mathbf{i} \) and its \( x \) coordinate \( h_k \), see the left panel of fig.3 for an example. During minimization of loss, we fix the normal of each weight and only tune its location. Furthermore, we fix the value of \( z_k \) and set \( z_k = 1 \) if \( \mathbf{n}_k = \mathbf{i} \) and \( z_k = -1 \) if \( \mathbf{n}_k = -\mathbf{i} \). As mentioned in subsection 4.3, the magnitude of \( z_k \) does not matter for identifying existence of genuine local minima. Fixing its sign amounts to choosing one of the two branches of local minima. Therefore, by the fact that \( \mathbf{w}_k \cdot \mathbf{x}_i \) is equal to the signed distance from \( \mathbf{x}_i \) to \( \mathbf{w}_k \), we have \( R_k \cdot \mathbf{x}_i = z_k \mathbf{w}_k \cdot \mathbf{x}_i = x_i - h_k \), where \( x_i = \mathbf{x}_i \cdot \mathbf{i} \).

The weights partition the input space into a series of regions, such as the \( \Omega_1, \Omega_2 \) and \( \Omega_3 \) in fig.3. Each region lies between two adjacent weight vectors, and in each region \( \Omega_j \), \( I_{k} (i \in \Omega_j) \) have constant values, which we denote as \( I_{\Omega_j,k} \). The total loss can be written as

\[
L = \sum_{\Omega_j} \sum_{i \in \Omega_j} \left( \sum_k I_{\Omega_j,k} x_i - \sum_k I_{\Omega_j,k} h_k - y_i \right)^2. \tag{20}
\]

By the assumption that all weight vectors are parallel, we have reduced the original problem to a one-dimensional one, which will greatly simplify the computation of probability discussed later. By the global optimality conditions \( \frac{\partial L}{\partial h_k} = 0 \), we can derive the following linear system,

\[
F \mathbf{h} = \mathbf{f}, \quad \text{where} \quad \mathbf{h} = (h_1, h_2, \cdots, h_K)^T, \tag{21}
\]

and \( F, \mathbf{f} \) are matrix and vector respectively with the following elements,

\[
F(l, k) = \sum_{\Omega_j} I_{\Omega_j,l} I_{\Omega_j,k} N_j, (l, k = \in [K]),
\]

\[
f(l) = \sum_{k} \sum_{\Omega_j} I_{\Omega_j,l} I_{\Omega_j,k} \sum_{i \in \Omega_j} x_i - \sum_{\Omega_j} I_{\Omega_j,l} \sum_{i \in \Omega_j} y_i. \tag{22}
\]

\( N_j \) is the number of samples in region \( \Omega_j \).

Let us first discuss the simple case of two weight vectors, with directions shown in the right panel of fig.3. The analytical solution to the linear system (21) can be easily obtained in this setting. (21) becomes

\[
\begin{pmatrix} N_1 & 0 & 0 \\ 0 & N_3 \\ 0 & N_3 \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} = \begin{pmatrix} N_{1+} \bar{x}_{1+} + N_{1-} \bar{x}_{1-} - N_{1+} + N_{1-} \\ N_{3+} \bar{x}_{3+} + N_{3-} \bar{x}_{3-} - N_{3+} + N_{3-} \end{pmatrix}, \tag{23}
\]

Figure 3: Computing the probability of existing local minima when all weight vectors are parallel.
where $N_{1+}$ is the number of positive examples in region $\Omega_1$, $\bar{x}_{1+}$ is the average of $x$ coordinates for all positive samples in $\Omega_1$, and so on. Assuming positive and negative classes have equal priors (thus the numbers of positive and negative samples are equal), and denoting the probability of positive (negative) examples lying in region $\Omega_j$ as $P_{j+}$ ($P_{j-}$), the solution to (23) is as follows

$$x_{w_1} = h_1 = \frac{P_{1+} \bar{x}_{1+} + P_{1-} \bar{x}_{1-} - P_{1+} + P_{1-}}{P_{1+} + P_{1-}},$$

$$x_{w_2} = h_2 = \frac{P_{3+} \bar{x}_{3+} + P_{3-} \bar{x}_{3-} - P_{3+} + P_{3-}}{P_{3+} + P_{3-}}, \quad (24)$$

where $x_{w_1}$ is the $x$ coordinate of $w_1$.

If there are more than two weight vectors, we need to solve the linear system (21) with $F$ and $f$ expressed in $P_{j+}, P_{j-}, \bar{x}_{j+}, \bar{x}_{j-}$ etc. See Appendix E.1 for the details.

### 7.2 Probability of Getting Trapped in Differentiable Local Minima for Gaussian Input Data

Now, assume data samples are drawn from Gaussian distribution. This implies $P_{j+} \neq 0$, $P_{j-} \neq 0$ in each finite region. As a result, $F$ will have full-rank and (21) will have a unique solution.

There exist gaps between $w_1^*$ and $w_1$, $w_2^*$ and $w_2$ respectively. If no samples lie in these gaps, then there will be a genuine local minimum into which local search methods will be stuck when starting from $\{w_1, w_2\}$. Therefore, suppose $N$ samples are i.i.d. drawn, the probability of existing local minima is

$$P_t = (1 - P_g)^N \quad (25)$$

where $P_g$ is the probability of a sample lying in one of the gaps. Use $g_1, g_2, ..., g_K$ to donate the gap regions,

$$P_g = P(x \in g_1 \cup g_2 \cdots \cup g_K). \quad (26)$$

For Gaussian distribution, the detailed analytical calculations of $P_g$, and $P_{j+}, P_{j-}, \bar{x}_{j+}, \bar{x}_{j-}$ on which it relies, are given in Appendix E.2.

Since $P_t$ is exponentially vanishing, the probability of existing local minima is very small as long as one of the gaps is large enough to have unnegligible probability of having samples in it. This conclusion still holds for weight vectors that are not parallel and data drawn from other distributions, due to the fact $w_1^*$ and $w_1$ usually forms an intermediate region in which the probability of having samples is nonzero.

The probabilities of existing saddle points and non-differentiable local minima are still exponentially vanishing because the gaps usually exist.

### 7.3 Experimental Results

In this subsection, we perform experiments to show how big the probability of getting stuck in differentiable local minima is and how it varies with the locations of weight vectors. The data distribution is shown in the right panel of fig.3. Both positive and negative samples are drawn from symmetrical multivariate Gaussian distribution, with means locating at $x_+ = 1$ and $x_- = -1$ respectively. Covariance matrices of both distributions are set as the identify matrix. $N$ is set to 100.

In the first experiment, we consider the case of two weight vectors: $w_1$ and $w_2$. At first, we fix $x_{w_1} = 0$ and move $w_1$ in the interval $[0,6]$. Fig.4(a) shows how a empirical loss changes with $x_{w_1}$, where there is clearly a global minimum and no bad local minima exist. We then use (24) to compute $x_{w_1}$ and $x_{w_2}$, and compute the probability of hitting local minima with (25). Fig.4(b) shows how this probability varies with $x_{w_1}$. Comparing fig.4(a) with fig.4(b), one can find that there is really a high probability of being trapped at the global minimum of loss, showing the correctness of our theory about the probability of getting stuck in local minima. When $x_{w_1}$ is far away from data means, this probability is close to 1 and the loss is almost constant, corresponding to getting trapped in flat plateau. This can be attributed to the fact that although there is still a gap between $x_{w_1}$ and $x_{w_2}$, the probability of samples lying in this gap is very low due to the exponentially vanishing nature of Gaussian density when moving away from data mean. The probability of hitting local minima is very low in other places in the weight space due to high probability of having samples in the gap.
Figure 4: The probability of existing local minima w.r.t. the locations of two weight vectors. (a) An empirical loss landscape when moving one of the weights. (b) The probability of existing local minima when moving one of the weights. (c) The probability of existing local minima when moving both weights.

We then consider the case in which both weights can move. Fig.4(c) shows the probability of getting stuck in local minima when moving both weights. It is actually the tensor product of the two probabilities for moving $x_{w_1}$ and $x_{w_2}$ independently. The small peak close to origin corresponds to the global minimum. The probability of getting trapped in bad local minima is very low if the weights are not too far away from data clusters. This may help to explain why the common practice of initializing weights randomly with small magnitudes succeeds when training neural networks.

Similar phenomena can be observed for the case of multiple weight vectors. We explore the case of four weight vectors in Appendix E.3. The results demonstrate that probability of getting trapped in bad local minima is still very low. Since for continuous Gaussian data distribution the concept of over-parameterization does not apply, it is not necessary to consider cases of much more weights.

Finally, we discuss the case of discrete data. If $F$ in (21) is rank deficient (some typical scenarios are discussed in Appendix E.1), the optimal locations of some weights are not unique and change freely. However, there are still gaps between remaining weights and their unique optimal solutions, thus there is a low probability of existing bad local minima. Things may be different for discrete data and over-parameterized networks. With increasing network size, more weights have free optimal locations and thus possible non-null intersections with their defining cells, leading to an increasing probability of existing bad local minima.

8 Conclusion and Future Work

we have studied the global loss landscape of one-hidden-layer ReLU networks, including the global-ness of differentiable local minima, the conditions for existing differentiable and non-differentiable local minima and saddle points, and the probability of existing bad local minima.

In our future work, we are interested in the following problems: 1) Borrow ideas from computational geometry and implement efficient intersection algorithms, and perform experiments on discrete data to identify the existence of bad local minima. 2) Global landscape of deep ReLU networks.

References

Allen-Zhu, Z., Li, Y., and Song, Z. A convergence theory for deep learning via over-parameterization. In International Conference on Machine Learning, 2019.

Choromanska, A., Mathieu, M. H. M., Arous, G. B., and LeCun, Y. The loss surfaces of multilayer networks. In Artificial Intelligence and Statistics, pp. 192–204, 2015.

Dauphin, Y. N., Pascanu, R., Gulcehre, C., Cho, K., Ganguli, S., and Bengio, Y. Identifying and attacking the saddle point problem in high-dimensional non-convex optimization. In Advances in Neural Information Processing Systems, 2014.

de Berg, M., Cheong, O., van Kreveld, M., and Overmars, M. Computational Geometry: Algorithms and Applications. Springer, 3rd edition, 2008.
Ding, T., Li, D., and Sun, R. Spurious local minima exist for almost all over-parameterized neural networks. *optimization online*, 2019.

Draxler, F., Veschgini, K., Salnhofer, M., and Hamprecht, F. A. Essentially no barriers in neural network energy landscape. In *International Conference on Machine Learning*, 2018.

Du, S. S. and Lee, J. D. On the power of over-parametrization in neural networks with quadratic activation. In *International Conference on Machine Learning*, 2018.

Du, S. S., Lee, J. D., Li, H., Wang, L., and Zhai, X. Gradient descent finds global minima of deep neural networks. In *International Conference on Machine Learning*, 2019.

Feizi, S., Javadi, H., Zhang, J., and Tse, D. Porcupine neural networks: (almost) all local optima are global. arXiv preprint arXiv:1710.02196, 2017.

Freeman, C. D. and Bruna, J. Topology and geometry of half-rectified network optimization. In *International Conference on Learning Representations*, 2017.

Gao, W., Makkuva, A. V., Oh, S., and Viswanath, P. Learning one-hidden-layer neural networks under general input distributions. arXiv preprint arXiv:1810.04133, 2018.

Garipov, T., Izmailov, P., Podoprikhin, D., Vetrov, D. P., and Wilson, A. G. Loss surfaces, mode connectivity, and fast ensembling of dnns. In *Advances in Neural Information Processing Systems*, 2018.

Ge, R., Lee, J. D., and Ma, T. Matrix completion has no spurious local minimum. In *Advances in Neural Information Processing Systems*, pp. 2973—2981, 2016.

Ge, R., Lee, J. D., and Ma, T. Learning one-hidden-layer neural networks with landscape design. arXiv preprint arXiv:1711.00501, 2017.

Goodfellow, I. J., Vinyals, O., and Saxe, A. M. Qualitatively characterizing neural network optimization problems. In *International Conference on Learning Representations*, 2015.

Hardt, M. and Ma, T. Identity matters in deep learning. In *International Conference on Learning Representations*, 2017.

Horn, R. A. and Johnson, C. R. *Matrix Analysis*. Cambridge University Press, 2012.

Jin, C., Ge, R., Netrapalli, P., Kakade, S. M., and Jordan, M. I. How to escape saddle points efficiently. In *Proceedings of the 34th International Conference on Machine Learning*, pp. 1724—1732, 2017.

Kawaguchi, K. Deep learning without poor local minima. In *Advances in Neural Information Processing Systems*, pp. 586—594, 2016.

Kawaguchi, K. and Bengio, Y. Depth with nonlinearity creates no bad local minima in resnets. arXiv preprint arXiv:110.09038, 2018.

Kawaguchi, K. and Kaelbling, L. P. Elimination of all bad local minima in deep learning. arXiv preprint arXiv:1901.00279, 2019.

Laurent, T. and von Brecht, J. H. Deep linear networks with arbitrary loss: All local minima are global. In *International Conference on Machine Learning*, 2018a.

Laurent, T. and von Brecht, J. H. The multilinear structure of relu networks. In *International Conference on Machine Learning*, 2018b.

Li, D., Ding, T., and Sun, R. On the benefit of width for neural networks: Disappearance of bad basins. arXiv preprint arXiv:1812.11039, 2018a.

Li, H., Xu, Z., Taylor, G., Studer, C., and Goldstein, T. Visualizing the loss landscape of neural nets. In *Advances in Neural Information Processing Systems*, 2018b.

Liang, S., Sun, R., Lee, J. D., and Srikant, R. Adding one neuron can eliminate all bad local minima. In *Advances in Neural Information Processing Systems*, 2018a.
Liang, S., Sun, R., Li, Y., and Srikant, R. Understanding the loss surface of neural networks for binary classification. In International Conference on Machine Learning, 2018b.

Liao, Q. and Poggio, T. Theory of deep learning ii: Landscape of the empirical risk in deep learning. arXiv preprint arXiv:1703.09833, 2017.

Lu, H. and Kawaguchi, K. Depth creates no bad local minima. arXiv preprint arXiv:1702.08580, 2017.

Mei, S., Bai, Y., and Montanari, A. The landscape of empirical risk for non-convex losses. In arXiv preprint, pp. arXiv:1607.06534, 2016.

Nguyen, Q. and Hein, M. On connected sublevel sets in deep learning. In International Conference on Machine Learning, 2019.

Nguyen, Q., Mukkamala, M. C., and Hein, M. On the loss landscape of a class of deep neural networks with no bad local valleys. In International Conference on Learning Representations, 2019.

Nouiehed, M. and Razaviyayn, M. Learning deep models: Critical points and local openness. arXiv preprint arXiv:1803.02968, 2018.

Pennington, J. and Bahri, Y. Geometry of neural network loss surfaces via random matrix theory. In International Conference on Machine Learning, 2017.

Pennington, J. and Worah, P. The spectrum of the fisher information matrix of a single-hidden-layer neural network. In Advances in Neural Information Processing Systems, 2018.

Safran, I. and Shamir, O. On the quality of the initial basin in overspecified neural networks. In International Conference on Machine Learning, pp. 774–782, 2016.

Safran, I. and Shamir, O. Spurious local minima are common in two-layer relu neural networks. In Proceedings of the 35 th International Conference on Machine Learning, 2018.

Shamir, O. Are resnets provably better than linear predictors? In Advances in Neural Information Processing Systems, 2018.

Soltanolkotabi, M., Javanmard, A., and Lee, J. D. Theoretical insights into the optimization landscape of overparameterized shallow neural networks. IEEE Transactions on Information Theory, 65(2): 742–769, 2019.

Soudry, D. and Carmon, Y. No bad local minima: Data independent training error guarantees for multilayer neural networks. In arXiv preprint, pp. arXiv:1605.08361, 2016.

Soudry, D. and Hoffer, E. Exponentially vanishing suboptimal local minima in multilayer neural networks. In arXiv preprint, pp. arXiv:1702.05777, 2017.

Swirszcz, G., Czarnecki, W. M., and Pascanu, R. Local minima in training of deep networks. arXiv preprint arXiv:1611.06310, 2016.

Venturi, L., Bandeira, A., and Bruna, J. Spurious valleys in two-layer neural network optimization landscapes. arXiv preprint arXiv:1802.06384, 2018.

Yun, C., Sra, S., and Jadbabaie, A. Global optimality conditions for deep neural networks. In International Conference on Learning Representations, 2018.

Yun, C., Sra, S., and Jadbabaie, A. Small nonlinearities in activation functions create bad local minima in neural networks. In International Conference on Learning Representations, 2019.

Zhang, L. Depth creates no more spurious local minima. arXiv preprint arXiv:1901.09827, 2019.

Zhou, P. and Feng, J. Empirical risk landscape analysis for understanding deep neural networks. In International Conference on Learning Representations, 2018.
Zhou, Y. and Liang, Y. Critical points of neural networks: Analytical forms and landscape properties. In *International Conference on Learning Representations*, 2018.

Zou, D., Cao, Y., Zhou, D., and Gu, Q. Stochastic gradient descent optimizes overparameterized deep relu networks. *arXiv preprint arXiv:1811.08888*, 2018.
Appendices

A. Proofs of Lemma 1 and Theorem 1

Lemma 1. Any differentiable local minimum of \( L(z, w) \) in \( \{z\} \) in main text corresponds to stationary point of \( L(R) \) in \( \{R\} \) in main text, i.e., \( \frac{\partial L}{\partial R_j} = 0 \) (\( j \in [K] \)).

Proof. The loss of one-hidden-layer ReLU networks is

\[
L(z_1, z_2, \ldots, z_K, w_1, w_2, \ldots, w_K) = \frac{1}{N} \sum_{i=1}^{N} \left( \sum_{j=1}^{K} z_j \cdot [w_j \cdot x_i]_+, y_i \right)
\]

(A.1)

After introducing variables \( I_{ij} \) and defining \( R_j = z_j \cdot w_j \), the loss is converted into

\[
L(R) \triangleq \frac{1}{N} \sum_{j=1}^{N} \left( \sum_{j=1}^{K} I_{ij} R_j \cdot x_i, y_i \right)
\]

(A.2)

where \( R = \{R_k, k \in [K]\} \).

At any differentiable local minimum \( \hat{z} = \{\hat{z}_k, k \in [K]\}, \hat{w}_k = \{\hat{w}_k, k \in [K]\} \), the derivatives \( \frac{\partial L}{\partial z_j}, \frac{\partial L}{\partial w_j} \) exist and are all equal to 0. By \( R_j = z_j \cdot w_j \) we have

\[
\frac{\partial L}{\partial z_j} (\hat{z}, \hat{w}) = \frac{\partial L}{\partial R_j} \left( \hat{R}_1, \hat{R}_2, \ldots, \hat{R}_j, \ldots, \hat{R}_K \right) \cdot \hat{w}_j = 0,
\]

(A.3)

\[
\frac{\partial L}{\partial w_j} (\hat{z}, \hat{w}) = \frac{\partial L}{\partial R_j} \left( \hat{R}_1, \hat{R}_2, \ldots, \hat{R}_j, \ldots, \hat{R}_K \right) \cdot \hat{z}_j = 0, \quad j \in [K],
\]

(A.4)

where \( \hat{R}_j = \hat{z}_j \cdot \hat{w}_j \). If \( \hat{z}_j \neq 0 \), (A.4) implies \( \frac{\partial L}{\partial R_j} = 0 \), and (A.3) will be satisfied automatically. If \( \hat{z}_j = 0 \), (A.4) is satisfied, we only need to prove \( \frac{\partial L}{\partial R_j} = 0 \) from (A.3) for the case \( \hat{z}_j = 0 \).

Since \( \{\hat{z}, \hat{w}\} \) is a local minima of \( L \), by definition, there exists \( \varepsilon > 0 \) such that for all \( w_j \) that satisfy \( \|w_j - \hat{w}_j\|_2 \leq \varepsilon \), the following holds

\[
L(\hat{z}_1, \hat{z}_2, \ldots, \hat{z}_K, \hat{w}_1, \hat{w}_2, \ldots, \hat{w}_j, \ldots, \hat{w}_K) \geq L(\hat{z}_1, \hat{z}_2, \ldots, \hat{z}_K, \hat{w}_1, \hat{w}_2, \ldots, \hat{w}_j, \ldots, \hat{w}_K).
\]

(A.5)

We now perturbate \( w_j \) to \( w_j' = w_j + \hat{z}_j u \), and keep \( \{\hat{z}_1, \hat{z}_2, \ldots, \hat{z}_K, \hat{w}_1, \hat{w}_2, \ldots, \hat{w}_j, \ldots, \hat{w}_K\} \) fixed, where \( u \in \mathbb{R}^d \) is an arbitrary unit vector. Notice that

\[
\hat{R}_j = \hat{z}_j \hat{w}_j = 0 \quad \text{and} \quad R_j' = \hat{z}_j w_j' = 0
\]

(A.6)

due to \( \hat{z}_j = 0 \). Therefore, loss \( L \) remains constant under this perturbation, that is,

\[
L(\hat{z}_1, \hat{z}_2, \ldots, \hat{z}_K, \hat{w}_1, \hat{w}_2, \ldots, \hat{w}_j', \ldots, \hat{w}_K) = L(\hat{z}_1, \hat{z}_2, \ldots, \hat{z}_K, \hat{w}_1, \hat{w}_2, \ldots, \hat{w}_j, \ldots, \hat{w}_K)
\]

(A.7)

It can be shown that \( \{\hat{z}_1, \hat{z}_2, \ldots, \hat{z}_K, \hat{w}_1, \hat{w}_2, \ldots, \hat{w}_j', \ldots, \hat{w}_K\} \) is still a local minimum of \( L \). For any \( w_j \) satisfying \( \|w_j - \hat{w}_j\|_2 \leq \frac{\varepsilon}{2} \), there is

\[
\|w_j - \hat{w}_j\|_2 \leq \|w_j - w_j'\|_2 + \|w_j' - \hat{w}_j\|_2 \leq \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon
\]

Then by (A.5) and (A.7), we get

\[
L(\hat{z}_1, \hat{z}_2, \ldots, \hat{z}_K, \hat{w}_1, \hat{w}_2, \ldots, \hat{w}_j', \ldots, \hat{w}_K) \geq L(\hat{z}_1, \hat{z}_2, \ldots, \hat{z}_K, \hat{w}_1, \hat{w}_2, \ldots, \hat{w}_j', \ldots, \hat{w}_K).
\]

(A.8)

This implies that \( \{z_1, z_2, \ldots, z_K, w_1, w_2, \ldots, w_j', \ldots, w_K\} \) is also a local minimum. As a result, similar to (A.3) we have

\[
\frac{\partial L}{\partial R_j} \left( \hat{R}_1, \hat{R}_2, \ldots, R_j', \ldots, \hat{R}_K \right) \cdot w_j' = 0
\]

(A.9)
Using the fact that $\hat{R}_j = R_j' = 0$ from (A.6) and consequently $\frac{\partial L}{\partial R_j} \left( \hat{R}_1, \hat{R}_2, \ldots, \hat{R}_j, \ldots \hat{R}_K \right) = \frac{\partial L}{\partial R_j} \left( \hat{R}_1, \hat{R}_2, \ldots, \hat{R}_j', \ldots \hat{R}_K' \right)$, subtracting (A.4) from (A.9) yields
\[
\frac{\partial L}{\partial R_j} \left( \hat{R}_1, \hat{R}_2, \ldots, \hat{R}_j, \ldots \hat{R}_K \right) \cdot u = 0.
\]
Since $u$ is arbitrary, this leads to $\frac{\partial L}{\partial R_j} \left( \hat{R}_1, \hat{R}_2, \ldots, \hat{R}_j, \ldots \hat{R}_K \right) = 0$. Therefore, no matter $z_j$ equals 0 or not, we always have $\frac{\partial L}{\partial R_j} = 0$, $(j \in [K])$ at local minima. This proof is inspired by [Laurent & Brecht, 2018a].

\[\square\]

**Lemma A1.** $L(R_1, R_2, \ldots R_K)$ is convex if $l$ is convex.

The convexity of $L(R_1, R_2, \ldots R_K)$ is proved by showing the positive definiteness of its Hessian. The proof is given in Appendix F.

Now, we are ready to prove the following Theorem 1 that establishes the globalness of differentiable local minima.

**Theorem 1.** If loss function $l$ is convex, then any differentiable local minimum of $L(z, w)$ is a global minimum. Furthermore, there are no local maxima for $L(z, w)$.

**Proof.** By Lemma 1, any differentiable local minimum of $L(z, w)$ is a stationary point of $L(R)$, which is its unique global minimum due to its convexity. Therefore, differentiable local minima are also global minima. Furthermore, similar to Lemma 1, one can prove that local maximum of $L(z, w)$ corresponds to local maximum of $L(R)$. However, the convexity of $L(R)$ means it has no local maximum. Therefore, there are no local maxima for $L(z, w)$.

\[\square\]

**B. An Illustrative Example of Landscape**

Suppose there is only one hidden neuron, and there are two samples in the two-dimensional input space: $x_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $x_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ with labels $y_1 = 1$, $y_2 = 1$. We set $z = 1$ and bias $b = 0$. Denoting the only weight vector as $w$, the two samples then become two vectors in the space of $w$, as shown in fig.A1.

There are in total four cells in the $w$ space. In cell $r_1$, $I_{11} = I_{21} = 0$, thus $A = 0$ and $R^*$ is arbitrary. According to (9) in the main text, the loss $L = \frac{1}{2} \left( y_1^2 + y_2^2 \right) = 1$. Actually, in cell $r_1$, both samples are not active and the loss does not change with $w$, thus the landscape is a flat plateau. Cell $r_2$ and $r_3$ are similar, and we will take $r_3$ as an example. In $r_3$, $I_{11} = 1$, $I_{21} = 0$, hence $A = \begin{pmatrix} x_1^T \\ 0 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $R^* = A^+ y + (I - A^+ A) c = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 1 \\ c_2 \end{pmatrix}$, which is a line with distance 1 from $x_1$. The minimal loss in $r_3$ is $L = \frac{1}{2}$. In region $r_4$, $I_{11} = I_{21} = 1$, $A = \begin{pmatrix} x_1^T \\ x_2^T \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$, thus $A^+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, R^* = y = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, indicating the landscape in $r_4$ has a unique minimum. The minimal loss in $r_4$ is $L = 0$ by (9) in the main text, hence the local minimum in $r_4$ is the global minimum.

**C. Necessary and Sufficient Conditions for Existence of Differentiable Saddle Points**

**C.1 Proof of Theorem 2**

**Theorem 2.** For the loss in (1) in main text with $l$ being the squared loss, there exist differentiable saddle points for all combinations of the form $(j_1, j_2, \ldots, j_K'; K' < K)$, where $(j_1, j_2, \ldots, j_K)$ is
any permutation of \(1, 2, \cdots, K\), and the optimal \(\{\mathbf{R}_j^* \ (j = j_1, j_2, \cdots, j_K')\}\) of saddle points are the solutions to the linear system

\[
\mathbf{B} \mathbf{\tilde{R}} = \mathbf{b}
\]

(C.1)

where \(\mathbf{\tilde{R}} = (\mathbf{R}_{j_1}^T, \mathbf{R}_{j_2}^T, \cdots, \mathbf{R}_{j_K'}^T)^T, \mathbf{B} \in \mathbb{R}^{K'd \times K'd}\) is a block matrix and \(\mathbf{b} \in \mathbb{R}^{K'd}\) is a block vector with the following components,

\[
\mathbf{B} \ (j, k) = \sum_{i=1}^{N} I_{ij} x_i \cdot I_{ik} x_i^T
\]

(C.2)

\[
\mathbf{b} \ (j) = \sum_{i=1}^{N} I_{ij} y_i, \ j, k = j_1, j_2, \cdots, j_K'.
\]

(C.3)

Optimal \(\{\mathbf{R}_j^* \ (j = j_{K'+1}, \cdots, j_K)\}\) of saddle points satisfy

\[
\sum_{i=1}^{N} e_i I_{ij} x_i \cdot \mathbf{w}_j^* = 0, \ j = j_{K'+1}, \cdots, j_K,
\]

(C.4)

where the error \(e_i = \sum_{k=j_1}^{j_{K'}} I_{ik} \mathbf{R}_k^* \cdot x_i - y_i\).

Proof. Since saddle points are stationary points, (A.3) and (A.4) still hold. If \(\frac{\partial L}{\partial \mathbf{R}_j} = 0\), (A.3) and (A.4) are both satisfied. On the other hand, \(z_j = 0\) if \(\frac{\partial L}{\partial \mathbf{R}_j} \neq 0\) by (A.4). However, \(\frac{\partial L}{\partial \mathbf{R}_j} \ (j = 1, 2, \cdots, K)\) can not all equal zero at the same time, otherwise the solutions would be differentiable local minima rather than saddle points. Without loss of generality, suppose \(\frac{\partial L}{\partial \mathbf{R}_j} = 0 \ (j = j_1, j_2, \cdots, j_{K'}; K' < K)\), and the remaining \(\frac{\partial L}{\partial \mathbf{R}_j} \ (j = j_{K'+1}, \cdots, j_K)\) are non-zero. We need to test all possible combinations \((j_1, j_2, \cdots, j_{K'})\) such that \(\frac{\partial L}{\partial \mathbf{R}_j} = 0 \ (j = j_1, j_2, \cdots, j_{K'}; K' < K)\), and see whether there exist saddle points.

Ignoring the factor \(\frac{1}{N}\) in \(L\) from now on, we have

\[
\frac{\partial L}{\partial \mathbf{R}_j} = 0 = \sum_{i=1}^{N} \left( \sum_{k=1}^{K} I_{ik} \mathbf{R}_k \cdot x_i - y_i \right) \cdot I_{ij} x_i, \ j = j_1, j_2, \cdots, j_{K'}.
\]

(C.5)

Since \(\frac{\partial L}{\partial \mathbf{R}_k} \neq 0 \ (k = j_{K'+1}, \cdots, j_K)\), by \(\mathbf{R}_k = 0\) due to associated \(z_k = 0\), we get

\[
\sum_{i=1}^{N} \left( \sum_{j=k}^{j_{K'}} I_{ik} x_i^T \mathbf{R}_k^* - y_i \right) \cdot I_{ij} x_i = 0, \ j = j_1, j_2, \cdots, j_{K'}
\]

(C.6)

Let \(\mathbf{\tilde{R}} = (\mathbf{R}_{j_1}^T, \mathbf{R}_{j_2}^T, \cdots, \mathbf{R}_{j_{K'}}^T)^T\), (C.6) leads to the following linear system

\[
\mathbf{B} \mathbf{\tilde{R}} = \mathbf{b}
\]
where \( \mathbf{B} \in \mathbb{R}^{K'd \times K'd} \) is a block matrix and \( \mathbf{b} \in \mathbb{R}^{K'd} \) is a block vector with components as shown in the theorem. The linear system is always solvable due to \( \mathbf{B} \) is a square matrix, and the general solution is

\[
\mathbf{R}^* = \mathbf{B}^+ \mathbf{b} + \left( \mathbf{I} - \mathbf{B}^+ \mathbf{B} \right) \mathbf{c} \quad (\mathbf{c} \in \mathbb{R}^{K'd} \text{ is arbitrary}). \tag{C.7}
\]

\( \hat{\mathbf{R}}^* \) can be a single point, the whole \( \mathbb{R}^{K'd} \) sapce or a linear subspace in \( \mathbb{R}^{K'd} \), corresponding to \( \text{rank}(\mathbf{B}) = K'd, \ (\mathbf{I} - \mathbf{B}^+ \mathbf{B}) \) is of full rank or not respectively.

For \( j = j_{K'^{+1}}, \cdots , j_K \) with \( \frac{\partial L}{\partial \mathbf{R}^*} \neq 0 \), (A.3) should be satisfied, resulting in

\[
\sum_{i=1}^{N} \left( \sum_{k=j_1}^{j_{K'}} I_{ik} \mathbf{R}_k^* \mathbf{x}_i - y_i \right) I_{ij} \mathbf{x}_i \cdot \mathbf{w}_j^* = 0
\]

Defining error \( e_i = \sum_{k=j_1}^{j_{K'}} I_{ik} \mathbf{R}_k^* \mathbf{x}_i - y_i \), we have

\[
[\sum_{i=1}^{N} e_i I_{ij} \mathbf{x}_i] \cdot \mathbf{w}_j^* = 0, \quad j = j_{K'^{+1}}, \cdots , j_K
\]

Therefore, \( \mathbf{w}_j^* \) is on a hyperplane that passes the origin in the space of \( \mathbf{w}_j \). (C.7) and (C.4) constitutes the necessary conditions that saddle points \((z, \mathbf{w}^*)\) must satisfy.

Now we proceed to prove that (C.7) and (C.4) are also sufficient for the existence of saddle points. Our approach is to prove that there exist both ascent and descent directions at these points. For any \( k \) that satisfies \( \frac{\partial L}{\partial \mathbf{R}_k^*} \neq 0 \) (thus \( z_k = 0 \)), we perturbate \( z_k \) and \( \mathbf{w}_k^* \) respectively as follows:

\[
0 \to \delta z_k, \ \mathbf{w}_k^* \to \mathbf{w}_k^* + \delta \mathbf{w}_k
\]

The loss function \( L \) after perturbation is

\[
L' = \sum_{i=1}^{N} \left( \sum_{j=j_1}^{j_{K'}} I_{ij} \mathbf{R}_j^* \mathbf{x}_i + I_{ik} \delta z_k \cdot (\mathbf{w}_k^* + \delta \mathbf{w}_k) \cdot \mathbf{x}_i - y_i \right)^2
\]

\[
= \sum_{i=1}^{N} \left( e_i + I_{ik} \delta z_k \cdot (\mathbf{w}_k^* + \delta \mathbf{w}_k) \cdot \mathbf{x}_i \right)^2 \tag{C.8}
\]

\[
= L + 2 \sum_{i=1}^{N} e_i I_{ik} \mathbf{w}_k^* \cdot \mathbf{x}_i \delta z_k + 2 \sum_{i=1}^{N} e_i I_{ik} \delta z_k \delta \mathbf{w}_k \cdot \mathbf{x}_i + \sum_{i=1}^{N} I_{ik} \delta z_k^2 (\mathbf{w}_k^* \cdot \mathbf{x}_i)^2,
\]

where we have used \( I_{ik}^2 = I_{ik} \) and ignored terms higher than 2nd-order. Applying (C.4), we get

\[
\Delta L = L' - L = 2 \sum_{i=1}^{N} e_i I_{ik} \delta z_k \mathbf{w}_k \cdot \mathbf{x}_i + \sum_{i=1}^{N} I_{ik} \delta z_k^2 (\mathbf{w}_k^* \cdot \mathbf{x}_i)^2 \tag{C.9}
\]

Only 2nd-order terms remains in (C.9). If \( \delta z_k \) is very small and \( \delta \mathbf{w}_k \) not too small, we only need to consider the term \( \sum_{i=1}^{N} e_i I_{ik} \delta z_k \delta \mathbf{w}_k \cdot \mathbf{x}_i \). Notice that \( I_{ik} \) can not be zero for all \( i \in [N] \), otherwise \( \frac{\partial L}{\partial \mathbf{R}_k} = 0 \) by (C.5), contradicting our assumption that \( \frac{\partial L}{\partial \mathbf{R}_k} \neq 0 \). Therefore, setting \( \delta z_k > 0 \), we can make \( \Delta L \geq 0 \) by setting \( \sum_{i=1}^{N} e_i I_{ik} \mathbf{x}_i \cdot \delta \mathbf{w}_k \geq 0 \) with appropriate \( \delta \mathbf{w}_k \), indicating both ascent and descent directions exist at \((z, \mathbf{w}^*)\), hence being saddle points.

\( \square \)

### C.2 Conditions for Existence of Genuine Differentiable Saddle Points

Like differentiable local minima, differentiable saddle points found by (C.7) and (C.4) may be outside their defining cells. The criteria for existence of genuine saddle points can be derived in a similar way as those for differentiable locail minima. The main difference with differentiable local minima is that although \( \hat{\mathbf{R}}^* \) can be a single point, whole space or a linear subspace, \( \mathbf{w}_j^* \ (j = j_{K'^{+1}}, \cdots , j_K) \) are on hyperplanes and hence we need to test their intersections with corresponding defining cells. Only when all \( \mathbf{w}_j^* \ (j = 1, 2, \cdots , K) \) are inside their defining cells, there exist genuine differentiable saddle points.
D. Non-differentiable Local Minima

D.1 Proofs of Lemma 2 and Theorem 3

Lemma 2. Suppose \( \bar{w}_m \) lies on the boundary of cell 1 and cell 2 separated by a sample \( x_n \), where cell 2 is on the positive side of \( x_n \) and cell 1 on negative side. \( \bar{w}_m \) is a non-differentiable minimum if and only if

\[
\left( \lim_{\bar{w}_m \to w_m} \frac{\partial L}{\partial w_m} |1\right) / |(-x_n)\) and \( \left( \lim_{\bar{w}_m \to w_m} \frac{\partial L}{\partial w_m} |2\right) / |x_n), \tag{D.1}
\]

where \( a//b \) denotes vectors \( a \) and \( b \) are in the same directions, \( \frac{\partial L}{\partial w_m} |1\) means \( \frac{\partial L}{\partial w_m} \) in cell 1.

In other words, at the non-differentiable local minima, \( \frac{\partial L}{\partial w_m} |1\) and \( \frac{\partial L}{\partial w_m} |2\) are perpendicular to the hyperplane of \( x_n \) and have opposite directions. Since \( L \) is indifferentiable w.r.t. \( w_m \) at \( \bar{w}_m \), we use the limit.

![A non-differentiable local minimum \( w_m \) lying on cell boundary defined by a sample \( x_n \).](image)

Proof of Lemma 2. By 1st-order Taylor expansion, \( L(\bar{w}_m + \Delta w_m) = L(\bar{w}_m) + \frac{\partial L}{\partial w_m}(\bar{w}_m) \cdot \Delta w_m \). Here we omit other variables in \( L \) and only perturbate \( w_m \). If \( \bar{w}_m \) is a local minima, any perturbation \( \Delta w_m \) should cause \( L \) to increase, i.e., \( \frac{\partial L}{\partial w_m}(\bar{w}_m) \cdot \Delta w_m \geq 0 \). If \( \frac{\partial L}{\partial w_m} |2 \) \( \bar{w}_m \) is not in the direction of \( x_n \), we can always find \( \Delta w_m \) that satisfies \( \frac{\partial L}{\partial w_m} |2 \) \( \bar{w}_m \) \( \Delta w_m < 0 \), such as either \( \Delta w_1 \) or \( \Delta w_2 \) in fig. A2, indicating descent directions exist in cell 2 and contradicting the assumption that \( \bar{w}_m \) is a local minima. Therefore, we have \( \frac{\partial L}{\partial w_m} |2 |x_n, \frac{\partial L}{\partial w_m} |1 |(-x_n) \) can be proved in a similar way.

On the other hand, if (D.1) holds, any \( \Delta w_m \) will increase or keep the loss by \( \frac{\partial L}{\partial w_m} \bar{w}_m \bar{w}_m \cdot \Delta w_m \geq 0 \). Therefore, (D.1) is sufficient for \( \bar{w}_m \) to be a local minima.

Theorem 3. For the loss in (1) in main text with \( l \) being the squared loss, there exist non-differentiable local minima that reside on the boundary of two cells if and only if the linear system \( DR = d \) has solutions for any \( m \in [K] \), where \( R = (R^T_1, R^T_2, \cdots, R^T_K)^T \), \( D \in \mathbb{R}^{(K+1)d \times Kd} \) is a matrix with the following block components

\[
D (j, k) = \sum_i I_{ij} I_{ik} x_i x_i^T \quad (j, k \in [K]; j \neq m),
\]

\[
D (m, k) = \sum_{i \neq n} I_{im} I_{ik} (x_i \cdot x_n x_n - |x_n|^2 x_i) x_i^T \quad (k \in [K]) \tag{D.2}
\]

\[
D (K + 1, m) = x_n^T, \quad D (K + 1, k) = 0 \quad (k \in [K]; k \neq m),
\]

and \( d \in \mathbb{R}^{(K+1)d} \) is a block vector,

\[
d (j) = \sum_i I_{ij} y_i x_i \quad (j \in [K]; j \neq m)
\]

\[
d (m) = \sum_{i \neq n} I_{im} y_i \left( x_i \cdot x_n x_n - |x_n|^2 x_i \right), \quad d (K + 1) = 0 \tag{D.3}
\]
and its solution $R^*$ satisfies the following two inequalities for either $z_m > 0$ or $z_m < 0$.

$$\sum_{i \neq n} \left[ (\sum_k I_{ik} R_k \cdot x_i - y_i) I_{im} x_i \cdot x_n \right] z_m < 0, \quad (D.4)$$

$$\sum_{i \neq n} \left[ (\sum_k I_{ik} R_k \cdot x_i - y_i) I_{im} x_i \cdot x_n \right] z_m + \left[ (\sum_k I_{nk} R_k \cdot x_n - y_n) x_n \right] z_m > 0. \quad (D.5)$$

**Proof.** At non-differentiable local minima, we have

$$\frac{\partial L}{\partial z_j} = \frac{\partial L}{\partial w_j} = 0 \quad (j \in [K]: j \neq m) \quad (D.6)$$

$$\frac{\partial L}{\partial z_m} = 0, \quad (D.7)$$

due to these derivatives are well-defined. Similar to Lemma 1, (D.6) leads to

$$\frac{\partial L}{\partial R_j} = 0 \quad (j \in [K]: j \neq m) \quad (D.8)$$

$w_m$ is on the hyperplane of $x_n$ means

$$w_m \cdot x_n = 0. \quad (D.9)$$

Now, (D.7), (D.8), (D.1) and (D.9) constitute the necessary and sufficient conditions for non-differentiable local minima. We will write them in detailed forms.

First, the derivatives $\frac{\partial L}{\partial w_m} |_1$ and $\frac{\partial L}{\partial w_m} |_2$ are

$$\frac{\partial L}{\partial w_m} |_1 = \sum_{i \neq n} \left[ (\sum_k I_{ik} R_k \cdot x_i - y_i) I_{im} x_i \right] \cdot z_m \quad (D.10)$$

$$\frac{\partial L}{\partial w_m} |_2 = \frac{\partial L}{\partial w_m} |_1 + \left[ (\sum_k I_{nk} R_k \cdot x_n - y_n) x_n \right] \cdot z_m \quad (D.11)$$

(D.7) yields

$$\sum_{i=1}^N \left[ (\sum_k I_{ik} R_k \cdot x_i - y_i) I_{im} x_i \right] \cdot w_m = 0 \quad (D.12)$$

This involves quadratic term of $w$. Fortunately, the left side of (D.12) is actually $\sum_{i=1}^N \frac{1}{z_m} \frac{\partial L}{\partial w_m} |_2 \cdot w_m$. Notice that $z_m \neq 0$, otherwise $\frac{\partial L}{\partial w_m} |_2 = 0$ by (D.10) and (D.11) and $w_m$ would have been treated as differentiable local minima. Combining (D.1) and (D.9), we conclude that (D.12) is satisfied automatically and impose no constraint at all.

(D.8) implies

$$\sum_{i=1}^N \left[ (\sum_k I_{ik} R_k \cdot x_i - y_i) I_{ij} x_i \right] = 0 \quad (j \in [K]: j \neq m) \quad (D.13)$$

(D.1) can be expressed as

$$\left( \frac{\partial L}{\partial w_m} |_1 \cdot x_n \right) x_n = \frac{\partial L}{\partial w_m} |_1 \cdot |x_n|^2 \quad (D.14)$$

and the inequalities

$$\frac{\partial L}{\partial w_m} |_1 \cdot x_n < 0, \quad \frac{\partial L}{\partial w_m} |_2 \cdot x_n > 0. \quad (D.15)$$
(D.14) indicates \( \frac{\partial L}{\partial w_m} \big|_1 \) is parallel to \( x_n \), so is \( \frac{\partial L}{\partial w_m} \big|_2 \) by (D.11). (D.15) ensures \( w_m \) is a local minima (and cannot be local maximum or saddle point). Considering \( z_m \neq 0 \), (D.14) can be written as the following linear form

\[
\sum_{i \neq n} \left[ \left( \sum_k I_{ik} R_k \cdot x_i - y_i \right) I_{im} \left( x_i \cdot x_n x_n \cdot x_i \right) - |x_n|^2 \right] = 0
\]

(D.16)

(D.9) can be transformed into

\[
x_n \cdot R_m = 0
\]

(D.17)

The inequalities (D.15) are expanded into

\[
\sum_{i \neq n} \left[ \left( \sum_k I_{ik} R_k \cdot x_i - y_i \right) I_{im} \cdot x_n \right] z_m < 0
\]

\[
\sum_{i \neq n} \left[ \left( \sum_k I_{ik} R_k \cdot x_i - y_i \right) I_{im} \cdot x_n \right] z_m + \left[ \left( \sum_k I_{ik} R_k \cdot x_n - y_n \right) |x_n|^2 \right] z_m > 0
\]

Now, (D.13), (D.16) and (D.17) together form a linear system as defined in the statement of this theorem,

\[
DR = d
\]

(D.18)

The linear system (D.18) have solutions if and only if

\[
DD^+ d = d
\]

(D.19)

If solvable, its general solution is

\[
R^* = D^+ d + (I - D^+ D) c \quad (c \in \mathbb{R}^{Kd} \text{ is arbitrary})
\]

(D.20)

If \( D \) is of full rank, then \( R^* = D^+ d \) is unique.

We need to test whether the solution in (D.20) satisfy the constraints imposed by inequalities (D.4) and (D.5). If \( R^* \) is a single point, substituting \( R^* = D^+ d \) into (D.4) and (D.5), then test against either \( z_m > 0 \) or \( z_m < 0 \). Only if (D.19) holds, and the inequalities hold for \( z_m > 0 \) or \( z_m < 0 \), there is a single point non-differentiable local minima. If \( R^* \) is a linear subspace of \( \mathbb{R}^{Kd} \), substituting (D.20) into (D.4) and (D.5), each inequality will define a half-space in \( \mathbb{R}^{Kd} \). For example, (D.4) transforms into

\[
\sum_{i \neq n} \left[ \left( \sum_k I_{ik} I_{im} x_i^T x_n x_n^T (I - D^+ D) \right)_k \right] z_m \cdot c - \sum_{i \neq n} \left[ I_{im} y_i x_i^T x_n \right] z_m + \sum_{i \neq n} \left[ \left( \sum_k I_{ik} I_{im} x_i^T x_n x_n^T (D^+ d) \right)_k \right] z_m < 0
\]

(D.21)

where \( (I - D^+ D) \) is the rows of \( (I - D^+ D) \) corresponding to \( R_k \), and so on.

\[\square\]

**D.2 Conditions for Existence of Genuine Non-differentiable Local Minima**

Like the case of differentiable local minima, existence of genuine non-differentiable local minima can be done by testing against (11) and (12) in the main text if \( R^* \) is unique, or finding intersections (like (13) in the main text) if \( R^* \) is a linear subspace. The differences with differentiable local minima lie in that there is no need to test \( w_n^* \) since it is constrained on the boundary, and the two inequalities (D.4) and (D.5) should be satisfied instead. If \( R^* \) is a linear subspace, the solutions to (13) in the main text, (D.4) and (D.5) can be obtained simultaneously by finding their common intersections.
E. Probability of Getting Trapped in Local Minima

E.1 Locations of Local Minima When All Weight Vectors Are Parallel

By the assumption that all weight vectors are parallel, we have derived the following linear system in the main text

\[ Fh = f \]  \hspace{1cm} (E.1)

where \( h = (h_1, h_2, \cdots, h_K)^T \), \( F \) is a symmetric matrix with the following elements

\[ F(l,k) = \sum_{\Omega_j} I_{\Omega_j} I_{\Omega_j} N_j, \quad l, k \in [K] \]  \hspace{1cm} (E.2)

where \( N_j \) is the number of samples in region \( \Omega_j \). \( f \) is a vector with components

\[ f(l) = \sum_k \sum_{\Omega_j} I_{\Omega_j} I_{\Omega_j} \sum_{i \in \Omega_j} x_i - \sum_{i \in \Omega_j} y_i, \quad l \in [K] \]  \hspace{1cm} (E.3)

Since \( F \) is a square matrix, (E.1) will have a unique solution if \( F \) is of full-rank. This situation corresponds to case 1) in section 4.1. If \( F \) is rank-deficient, some components in \( h \) can be free. This situation corresponds to case 2) in section 4.1, and two typical scenarios are as follows. a). No samples lie between two weights with the same normal directions, such as \( w_l \) and \( w_{l'} \) in fig. A3(a). The \( l \)th and \( l' \)th rows of \( F \) will be equal, leading to rank-deficient \( F \). This happens frequently for over-parameterized networks. b). There are no samples lie on the positive side of a weight vector, such as \( w_k \) shown in fig. A3(a). As a result, \( N_j = 0 \) for all regions \( \Omega_j \) with \( I_{\Omega_j} = 1 \), the \( k \)th row of \( F \) will be zeros, resulting in rank-deficient \( F \) as well. Such weights are not involved in the optimization and can have free locations. If no samples lie on the positive sides of all weights, as shown in fig. A3(b), we have \( F = 0 \), corresponding to a flat plateau in the landscape.

If there are more than two weight vectors, we need to solve the linear system (E.1), with the following \( F \) and \( f \) expressed in \( P_{j+}, P_{j-}, \bar{x}_{j+}, \bar{x}_{j-} \) (assume equal priors for positive and negative classes),

\[ F(l,k) = \sum_{\Omega_j} I_{\Omega_j} I_{\Omega_j} (P_{j+} + P_{j-}), \quad l, k \in [K], \]  \hspace{1cm} (E.4)

\[ f(l) = \sum_k \sum_{\Omega_j} I_{\Omega_j} I_{\Omega_j} (P_{j+} \bar{x}_{j+} + P_{j-} \bar{x}_{j-}) - \sum_{\Omega_j} I_{\Omega_j} (P_{j+} - P_{j-}) \quad l \in [K] \]  \hspace{1cm} (E.5)

E.2 Probability of Existing Local Minima for Gaussian Input Data

We assume that both positive and negative samples are multivariate Gaussian distribution, with \( x_+ = 1 \) and \( x_- = -1 \) respectively, where \( x_+ \) and \( x_- \) are the \( x \) coordinates of means. Covariance matrices for both classes are set as identity matrix. Therefore, the probability densities are as follows

\[ P_{\pm}(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_\pm)^2}{2}}, \quad \frac{1}{\sqrt{2\pi}} e^{-\frac{x_-^2}{2}}, \quad \frac{1}{\sqrt{2\pi}} e^{-\frac{x_+^2}{2}}, \quad \cdots, \quad \frac{1}{\sqrt{2\pi}} e^{-\frac{x_-^2}{2}} \]  \hspace{1cm} (E.6)
We use four weights whose initial locations are \([0.1, 0.05, 0, -0.05]\) respectively, then move these weights. We perform experiments to show the probability of existing differentiable local minima when there are multiple weight vectors and consequently multiple gaps, using \(g_i\) to donate the gap regions, we use \(\Phi(x)\) is the cumulative distribution function of standard Gaussian distribution \(N(0, 1)\).

When there are multiple weight vectors and how it varies with the locations of weights. Assuming equal priors for positive and negative samples, the probability of a sample lying in gap \(g_i\) is

\[
P(x \in g_i) = \frac{1}{2} \left[ P(x \in g_i \mid y = 1) + P(x \in g_i \mid y = -1) \right]
\]

\[
= \frac{1}{2} \left[ \int_{g_i} P_+ (x) dx + \int_{g_i} P_- (x) dx \right]
\]

\[
= \frac{1}{2} \left[ \int_{x_{w_i}}^{x_{w_i}^*} \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_+)^2}{2}} dx + \int_{x_{w_i}^*}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_-)^2}{2}} dx \right]
\]

\[
= \frac{1}{2} \left[ \Phi(x_{w_i}^* - x_+) - \Phi(x_{w_i} - x_-) + \Phi(x_{w_i}^* - x_-) - \Phi(x_{w_i} - x_-) \right]
\]

where \(x_{w_i}, x_{w_i}^*\) are the \(x\) coordinates of \(w_i\) and \(w_i^*\) respectively, \(\Phi(x)\) is the cumulative distribution function of standard Gaussian distribution \(N(0, 1)\).

When there are multiple weight vectors and consequently multiple gaps, using \(g_1, g_2, \ldots, g_K\) to donate the gap regions, we use \(\max_i P(x \in g_i)\) to approximate \(P_g\) (the probability of a sample lying in one of the gaps) because of

\[
P_g = P(x \in g_1 \cup g_2 \cdots \cup g_K) \geq \max_i P(x \in g_i)
\]

(E.8)

The quantities \(P_{j+}, P_{j-}, \bar{x}_{j+}, \bar{x}_{j-}\) for each region \(\Omega_j\) that appeared in (E.4) and (E.5) are computed as follows. As an example, using the Gaussian distributions in (E.6), we get,

\[
P_{1+} = \int_{x_{w_1}}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_+)^2}{2}} dx = \int_{x_{w_1} - x_+}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx = 1 - \Phi(x_{w_1} - x_+)
\]

(E.9)

Using truncated Gaussian distribution, we have

\[
\bar{x}_{1+} = \int_{x_{w_1}}^{\infty} x \cdot \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_+)^2}{2}} dx / \int_{x_{w_1}}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_+)^2}{2}} dx
\]

\[
= \left[ \int_{x_{w_1}}^{\infty} (x - x_+) \cdot \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_+)^2}{2}} dx + x_+ \int_{x_{w_1}}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_+)^2}{2}} dx \right] / [1 - \Phi(x_{w_1} - x_+)] + x_+
\]

(E.10)

\(P_{1-}, \bar{x}_{1-}\) can be obtained similarly. The quantities for other regions can be calculated in similar ways, using corresponding intervals for the integrals.

E.3 More Experimental Results

We perform experiments to show the probability of existing differentiable local minima when there are multiple weight vectors and how it varies with the locations of weights.

We use four weights whose initial locations are \([0.1, 0.05, 0, -0.05]\) respectively, then move these weights and solve (E.11) to get their optimal locations. Due to the hugeness of this 4-dimensional weight space, we only visualize some slices in it. For example, fig.A4(a) shows the probability of existing differentiable local minima when moving only the uppermost weight vector, and fig.A4(b) exhibits the case of moving all weight vectors simultaneously. These results demonstrate that probability of getting trapped in bad local minima is usually very low.

F. The Convexity of \(L(R_1, R_2, \cdots R_K)\)

Lemma A2. \(L(R_1, R_2, \cdots R_K)\) is convex if \(l\) is convex
Proof. We will prove the convexity of \( L(R_1, R_2, \cdots, R_K) \) by proving the positive definiteness of its Hessian. The derivative is \( \frac{\partial L}{\partial R_m} = \frac{1}{N} \sum_{i=1}^{N} l' \left( \sum_{j=1}^{K} I_{ij} R_j \cdot x_i, y_i \right) \cdot I_{im} x_i \) and the 2nd-order derivative is
\[
\frac{\partial^2 L}{\partial R_m \partial R_n} = \frac{1}{N} \sum_{i=1}^{N} l'' \cdot I_{im} x_i I_{in} x_i^T \tag{F.1}
\]
Let \( R = (R_1^T, R_2^T, \cdots, R_K^T)^T \), then Hessian matrix \( \frac{\partial^2 L}{\partial R^2} \) is a block matrix with block components \( \frac{\partial^2 L}{\partial R_m \partial R_n} \). Since \( I_{im} \) is either 1 or 0, (F.1) can be rewritten as
\[
\frac{\partial^2 L}{\partial R_m \partial R_n} = \frac{1}{N} \sum_{i=1}^{N} l'' \cdot \begin{pmatrix}
I_{im} \cdot x_{i1} \\
I_{im} \cdot x_{i2} \\
\vdots \\
I_{im} \cdot x_{id}
\end{pmatrix} \begin{pmatrix}
I_{in} \cdot x_{i1} \\
I_{in} \cdot x_{i2} \\
\vdots \\
I_{in} \cdot x_{id}
\end{pmatrix}^T \tag{F.2}
\]
Defining \( I_{im} = (I_{im} \quad I_{im} \quad \cdots \quad I_{im})^T \) that repeats \( I_{im} \) \( d \) times, and using the element-wise product \( \odot \),
\[
\begin{pmatrix}
I_{im} \cdot x_{i1} \\
I_{im} \cdot x_{i2} \\
\vdots \\
I_{im} \cdot x_{id}
\end{pmatrix} \odot \begin{pmatrix}
I_{im} \cdot x_{i1} \\
I_{im} \cdot x_{i2} \\
\vdots \\
I_{im} \cdot x_{id}
\end{pmatrix} = I_{im} \odot x_i \]
we have
\[
\frac{\partial^2 L}{\partial R_m \partial R_n} = \frac{1}{N} \sum_{i=1}^{N} l'' \cdot I_{im} \odot x_i \cdot (I_{im} \odot x_i)^T
\]
Let \( \tilde{x}_i = \begin{pmatrix}
I_{i1} \odot x_i \\
I_{i2} \odot x_i \\
\vdots \\
I_{iK} \odot x_i
\end{pmatrix} \), then Hessian \( \frac{\partial^2 L}{\partial R^2} \) can be transformed into
\[
\frac{\partial^2 L}{\partial R^2} = \frac{1}{N} \sum_{i=1}^{N} l'' \cdot \tilde{x}_i \cdot \tilde{x}_i^T
\]
For arbitrary non-zero vector \( u \in \mathbb{R}^{Kd} \), the quadratic form \( u^T \frac{\partial^2 L}{\partial R^2} u = \frac{1}{N} \sum_{i=1}^{N} l'' \cdot (u^T \tilde{x}_i)^2 \). By \( l'' > 0 \) due to convexity of \( l \), the positive definiteness of Hessian and consequently the convexity of \( L \) are followed.