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# Spurious Local Minima of Deep ReLU Neural Networks in the Neural Tangent Kernel Regime

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## Abstract

In this paper, we theoretically prove that the deep ReLU neural networks do not lie in spurious local minima in the loss landscape under the Neural Tangent Kernel (NTK) regime, that is, in the gradient descent training dynamics of the deep ReLU neural networks whose parameters are initialized by a normal distribution in the limit as the widths of the hidden layers tend to infinity.

## 1 Introduction

Hinton et al. proposed Deep Belief Networks with a learning algorithm that trains one layer at a time [1]. Since that report, deep neural networks have attracted attention extensively because of their human-like intelligence achieved through learning and generalization. To date, deep neural networks have produced outstanding results in the fields of image processing, speech recognition and machine translation [2–6]. Moreover, their scope of application has expanded, for example, to the field of mathematics [7].

**Local minima in neural networks.** On the one hand, local minima of neural networks have been investigated for a long time. Local minima cause plateaus which have a strong negative influence on learning in neural networks [8, 9]. Fukumizu et al. have mathematically proved that critical points introduced by a hierarchical structure in a three-layered neural network can be local minima or saddle points according to conditions [10]. Dauphin et al. experimentally investigated the distribution of the critical points of a single-layer MLP and demonstrated that the possibility of existence of local minima with large error (i.e., bad or spurious local minima) is very small [11]. Yun et al. investigated the loss surface of three-layered neural networks with the standard activation functions such as ReLU, Leaky ReLU, sigmoid, tanh, arctan, ELU and SELU, and constructively proved that there is a spurious local minimum [12]. As for deep neural networks, Choromanska et al. provided a theoretical justification for the work in [11] on a deep neural network with ReLU units using the spherical spin-glass model under seven assumptions [13]. Choromanska et al. also suggested that discarding the seven unrealistic assumptions remains an important open problem [14]. Kawaguchi discarded most of these assumptions and proved that the following four statements for a deep ReLU neural network with only two out of the seven assumptions [15]: 1) the loss function is non-convex and non-concave, 2) every local minimum is a global minimum, 3) every critical point that is not a global minimum is a saddle point, and 4) bad saddle points exist. Nitta showed that there exist a large number of critical points introduced by a hierarchical structure in deep neural networks as straight lines, and derived a sufficient condition for deep neural networks having no critical points introduced by a hierarchical structure [16]. Laurent et al. studied the loss surface of deep ReLU or Leaky ReLU neural networks applied to classification problems, and proved that there are only two types of local minima: flat minima and sharp minima. They clarified that the sharp minima are

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\*Part of this work has been done at the National Institute of Advanced Industrial Science and Technology.

spurious local minima, and that the flat minima are global minima in the case of the Leaky ReLU network [17]. Liu et al. constructively proved that there exist non-differentiable saddle points in the loss surface of deep ReLU networks with squared loss or cross-entropy loss, and that deep ReLU networks with cross-entropy loss have non-differentiable spurious local minima under a mild restriction on datasets [18]. Incidentally, Nitta investigated the characteristics of the complex-valued neuron model with parameters represented by polar coordinates and showed that singular points degrade the learning speed in the case of using the steepest gradient descent method with square error [19]. As for three-layered complex-valued neural networks, Nitta mathematically proved that most of local minima caused by the hierarchical structure can be resolved by extending the real-valued neural network to complex numbers [20].

**Neural Tangent Kernel.** On the other hand, it is proved that for a least-squares regression cost, the vector of the parameters of deep neural networks has the same distribution as the initial value of the vector of the parameters for all times in the Neural Tangent Kernel (NTK) regime where the vector of the parameters is initialized with a normal distribution, and the width of hidden layers is infinity [21]. Since then, theoretical research in the NTK regime has become active. Allen-Zhu et al. proved that the parameters of deep ReLU neural networks move little from their initial values during training such as stochastic gradient descent and used it to show the training algorithm can find global minima on the error function in polynomial time in the NTK regime [22]. Du et al. proved the same thing as in [22] for the case of Lipschitz and smooth activation functions such as the soft-plus and sigmoid [23]. Lee et al. theoretically showed that the learning dynamics with a certain learning rate in parameter space of deep nonlinear neural networks are exactly described by a linearized model where the parameters of the deep neural networks move little from their initial values in the NTK regime [24]. That is, the trained network is equivalent to a linearized model around random initialization. Karakida et al. analyzed the generalization performance of continual learning in the NTK regime [25].

**Results of this paper.** In this paper, by discarding the remaining two assumptions in [15], we prove that the deep ReLU neural networks do not lie in spurious local minima in the loss landscape under the NTK regime, that is, in the gradient descent training dynamics of the deep ReLU neural networks whose parameters are initialized by a normal distribution in the limit as the widths of the hidden layers tend to infinity.

## 2 Analysis on spurious local minima

In this section, we theoretically prove that the deep ReLU neural networks do not lie in spurious local minima in the loss landscape under the NTK regime.

### 2.1 Kawaguchi model

This subsection presents a description of the deep ReLU neural network model analyzed in [15] (we call it *Kawaguchi model* here).

First, we consider the following neuron. The net input  $U_n$  to a neuron  $n$  is defined as:  $U_n = \sum_m W_{nm} I_m$ , where  $W_{nm}$  represents the weight connecting the neurons  $n$  and  $m$ ,  $I_m$  represents the input signal from the neuron  $m$ . It is noteworthy that biases are omitted for the sake of simplicity.

The output signal is defined as  $\varphi(U_n)$  where  $\varphi(u) \stackrel{\text{def}}{=} \max(0, u)$  for any  $u \in \mathbb{R}$  and is called *Rectified Linear Unit (ReLU)*,  $\mathbb{R}$  denotes the set of real numbers).

The deep nonlinear neural network described in [15] consists of such neurons described above (Fig. 1). The network has  $H + 2$  layers ( $H$  is the number of hidden layers). The activation function  $\psi$  of the neuron in the output layer is linear, i.e.,  $\psi(u) = u$  for any  $u \in \mathbb{R}$ . For any  $0 \leq k \leq H + 1$ , let  $d_k$  denote the number of neurons of the  $k$ -th layer, that is, the width of the  $k$ -th layer where the 0-th layer is the input layer and the  $(H + 1)$ -th layer is the output layer. Let  $d_x = d_0$  and  $d_y = d_{H+1}$  for simplicity.

Let  $(\mathbf{X}, \mathbf{Y})$  be the training data where  $\mathbf{X} \in \mathbb{R}^{d_x \times m}$  and  $\mathbf{Y} \in \mathbb{R}^{d_y \times m}$  and where  $m$  denotes the number of training patterns. We can rewrite the  $m$  training data as  $\{(\mathbf{X}_i, \mathbf{Y}_i)\}_{i=1}^m$  where  $\mathbf{X}_i \in \mathbb{R}^{d_x}$  is the  $i$ -th input training pattern and  $\mathbf{Y}_i \in \mathbb{R}^{d_y}$  is the  $i$ -th output training pattern. Let  $\mathbf{W}_k$  denote the weight matrix between the  $(k - 1)$ -th layer and the  $k$ -th layer for any  $1 \leq k \leq H + 1$ . Let  $\Theta$

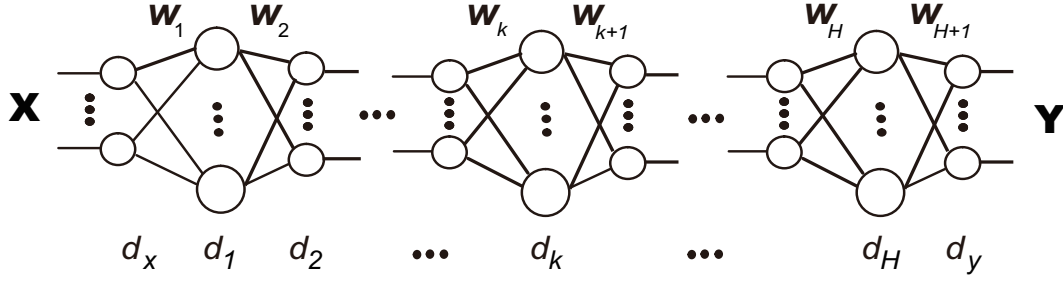


Figure 1: A deep neural network model [15]:  $(\mathbf{X}, \mathbf{Y})$  are the training data,  $\mathbf{W}_k$  signifies the weight matrix between the  $(k - 1)$ -th layer and the  $k$ -th layer, and  $d_k$  denotes the number of neurons of the  $k$ -th layer.

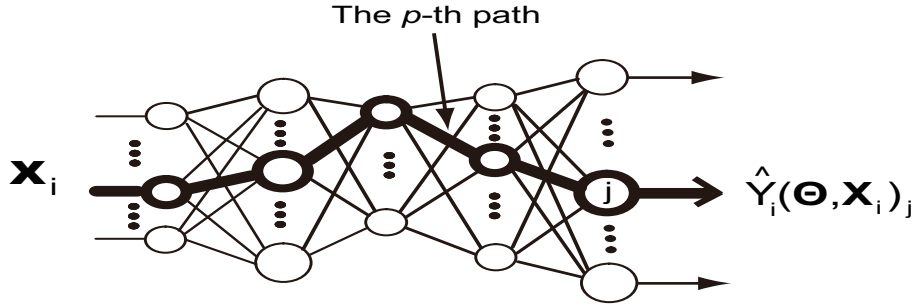


Figure 2: Image of a path in the deep neural network model [15]:  $\mathbf{X}_i$  denotes the  $i$ -th input training pattern, and  $\hat{Y}_i(\Theta, \mathbf{X}_i)_j$  stands for the actual output of output neuron  $j$ .

denote the one-dimensional vector which consists of all the weight parameters of the deep nonlinear neural network.

Kawaguchi specifically examined a path from an input neuron to an output neuron of the deep ReLU neural network (Fig. 2), and expressed the actual output of output neuron  $j$  of the output layer of the deep ReLU neural network for the  $i$ -th input training pattern  $\mathbf{X}_i \in \mathbb{R}^{d_x}$  as

$$\hat{Y}_i(\Theta, \mathbf{X}_i)_j = q \sum_{p=1}^{\Psi} [\mathbf{X}_i]_{(j,p)} [\mathbf{Z}_i]_{(j,p)} \prod_{k=1}^{H+1} w_{(j,p)}^{(k)} \in \mathbb{R} \quad (1)$$

where  $\Psi$  represents the total number of paths from the input layer to output neuron  $j$ ,  $[\mathbf{X}_i]_{(j,p)} \in \mathbb{R}$  denotes the component of the  $i$ -th input training pattern  $\mathbf{X}_i \in \mathbb{R}^{d_x}$  that is used in the  $p$ -th path to the  $j$ -th output neuron, and  $q$  is a constant for normalization. Also,  $[\mathbf{Z}_i]_{(j,p)} \in \{0, 1\}$  represents whether the  $p$ -th path to the output neuron  $j$  is active or not for each training pattern  $i$  as a result of ReLU activation.  $[\mathbf{Z}_i]_{(j,p)} = 1$  means that the path is active, and  $[\mathbf{Z}_i]_{(j,p)} = 0$  means that the path is inactive.  $w_{(j,p)}^{(k)} \in \mathbb{R}$  is the component of the weight matrix  $\mathbf{W}_k \in \mathbb{R}^{d_k \times d_{k-1}}$  that is used in the  $p$ -th path to the output neuron  $j$ .

The objective of the training is to find the parameters which minimize the error function defined as

$$L(\Theta) = \frac{1}{2} \sum_{i=1}^m E_{\mathbf{Z}} \|\hat{Y}_i(\Theta, \mathbf{X}_i) - \mathbf{Y}_i\|^2 \quad (2)$$

where  $\|\cdot\|$  is the Euclidean norm, that is,  $\|\mathbf{u}\| = \sqrt{u_1^2 + \dots + u_N^2}$  for a vector  $\mathbf{u} = (u_1 \dots u_N)^T \in \mathbb{R}^N$ , and  $\hat{Y}_i(\Theta, \mathbf{X}_i) \in \mathbb{R}^{d_y}$  is the actual output of the output layer of the deep nonlinear neural network for the  $i$ -th training pattern  $\mathbf{X}_i$ . The expectation in Eq. (2) is made with respect to random vector  $\mathbf{Z} = \{[\mathbf{Z}_i]_{(j,p)}\}$ .

The Kawaguchi model has been analyzed based on the following two assumptions.

**A1p-m**  $P([\mathbf{Z}_i]_{(j,p)} = 1) = \rho$  for all  $i$  and  $(j, p)$  where  $\rho \in \mathbb{R}$  is a constant. That is,  $[\mathbf{Z}_i]_{(j,p)}$  is a Bernoulli random variable.

**A5u-m**  $\mathbf{Z}$  is independent of the input  $\mathbf{X}$  and the parameter  $\Theta$ .

A1p-m and A5u-m are weaker ones of the two assumptions A1p and A5u in [13], respectively. The next corollary is one of the main results in [15].

**Corollary 1** (Kawaguchi, 2016: deep ReLU networks) Assume A1p-m and A5u-m. Let  $q = \rho^{-1}$ . Further, assume that  $\mathbf{X}\mathbf{X}^T$  and  $\mathbf{X}\mathbf{Y}^T$  are full rank, and  $d_y \leq d_x$ . Then, for any depth  $H \geq 1$  and for any layer widths and any input-output dimensions  $d_y, d_H, d_{H-1}, \dots, d_1, d_x \geq 1$ , the error function  $L(\Theta)$  has the following properties:

1. It is non-convex and non-concave.
2. Every local minimum is a global minimum.
3. Every critical point that is not a global minimum is a saddle point.
4. If  $\text{rank}(W_H \cdots W_2) = \min(d_H, \dots, d_1)$ , then the Hessian at any saddle point has at least one (strictly) negative eigenvalue.

□

Note that the assumptions on  $\mathbf{X}\mathbf{X}^T$  and  $\mathbf{X}\mathbf{Y}^T$  in Corollary 1 are realistic and easy to satisfy.

Strictly speaking, the following assumption A5u-m-1 suffices for the proof instead of the assumption A5u-m described above

**A5u-m-1** For any  $i$  and any  $(j, p)$ ,  $[\mathbf{Z}_i]_{(j,p)} \in \{0, 1\}$  is independent of the  $i$ -th input training pattern  $\mathbf{X}_i \in \mathbb{R}^{d_x}$  and the sequence of the weights on the  $p$ -th path  $\{w_{(j,p)}^{(k)} \in \mathbb{R}\}_{k=1}^{H+1}$  where  $w_{(j,p)}^{(k)}$  is the weight between the layer  $k-1$  and the layer  $k$  on the  $p$ -th path ( $k = 1, \dots, H+1$ ).

Actually, according to assumption A5u-m-1,

$$\begin{aligned}
& E_{\mathbf{Z}} \left[ \hat{\mathbf{Y}}_i(\Theta, \mathbf{X}_i)_j \right] \\
&= E_{\mathbf{Z}} \left[ q \sum_{p=1}^{\Psi} [\mathbf{X}_i]_{(j,p)} [\mathbf{Z}_i]_{(j,p)} \prod_{k=1}^{H+1} w_{(j,p)}^{(k)} \right] \quad (\text{from Eq.(1)}) \\
&= q \sum_{p=1}^{\Psi} [\mathbf{X}_i]_{(j,p)} E_{\mathbf{Z}} \left[ [\mathbf{Z}_i]_{(j,p)} \prod_{k=1}^{H+1} w_{(j,p)}^{(k)} \right]. \quad (\text{from the assumption A5u-m-1}) \quad (3)
\end{aligned}$$

Kawaguchi analyzed the deep ReLU neural network using Eq. (3) (see Section 3.2 in [15]).

## 2.2 Analysis

This subsection presents an analysis of the Kawaguchi model in the NTK regime.

**NTK regime.** First, we here summarize the NTK regime. Consider a fully connected deep neural network defined as

$$h_l = \phi(u_l), \quad (4)$$

$$u_l = \frac{\sigma_w W_l h_{l-1}}{\sqrt{M_{l-1}}} + \sigma_b b_l \quad (l = 1, \dots, L) \quad (5)$$

where  $\phi$  is an activation function,  $W_l \in \mathbb{R}^{M_l \times M_{l-1}}$  the weight matrix between the layer  $l-1$  and layer  $l$ ,  $b_l \in \mathbb{R}^{M_l}$  the bias of the layer  $l$ ,  $\sigma_w^2$  the variance of weights,  $\sigma_b^2$  the variance of biases, and  $M_l$  the number of neurons in the hidden layer  $l$ . Each element of the weight and the bias is initialized according to the normal distribution  $N(0, 1)$ . That is, we can assume that each weight is initialized according to the normal distribution  $N(0, \sigma_w^2/M_{l-1})$ . Then one discusses the behavior or properties of the deep neural network when  $M_l \rightarrow \infty$ , that is, the width of hidden layers goes to infinity. This is known as the NTK regime.

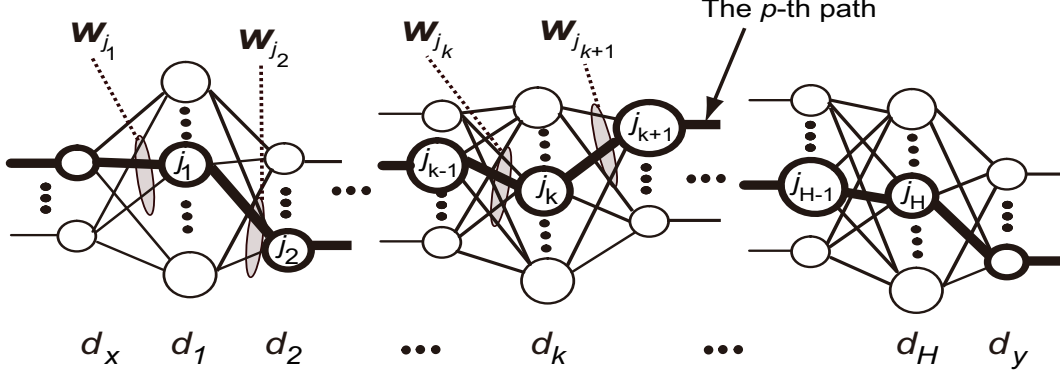


Figure 3: A deep ReLU neural network with  $H$  hidden layers where  $\mathbf{w}_{j_k}$  is the weight vector of hidden neuron  $j_k$ , hidden neurons  $j_1, \dots, j_H$  are on the  $p$ -th path,  $d_k$  is the number of neurons of the  $k$ -th layer,  $d_x = d_0$  and  $d_y = d_{H+1}$ .

**Kawaguchi model in the NTK regime.** We assume in this analysis that each weight between the layer  $l$  and the layer  $l + 1$  is set according to the normal distribution  $N(0, \sigma_l^2)$  where  $\sigma_l = 1/(3d_l)$  and  $d_l$  is the number of neurons in the layer  $l$ . We also assume that the width of the deep ReLU neural network is sufficiently large, that is,  $d_0 (= d_x), d_1, \dots, d_{H-1}$  are sufficiently large (Fig. 1), and that each element of the  $i$ -th input training pattern  $\mathbf{X}_i$  takes a value between  $-\alpha$  and  $\alpha$ , that is,  $\mathbf{X}_i \in I^{d_x}$  for any  $i$  where  $I = [-\alpha, \alpha]$  and  $\alpha$  is a positive real number. By adding these assumptions described above, we can regard that the Kawaguchi model is in the NTK regime, and call it the *Kawaguchi model in the NTK regime*.

Incidentally, in He initialization which is commonly used in practice, the initial value of each weight between the layer  $l$  and the layer  $l + 1$  is set according to either of the normal distributions  $N(0, 2/d_l)$  or  $N(0, 2/d_{l+1})$  independently [26]. Thus, the case of the He initialization is included in the Kawaguchi model in the NTK regime.

**Flow of analysis.** We prove in the following Theorems 1-3 that the two assumptions A1p-m and A5u-m (A5u-m-1) are satisfied in the initial state immediately after the parameter initialization of the Kawaguchi model in the NTK regime. Then, we will realize in Theorem 4 that the error function  $L(\Theta)$  does not lie in spurious local minima in the initial state immediately after the parameter initialization under the NTK regime according to Corollary 1. After that, we will prove in Theorem 5 that the error function  $L(\Theta)$  does not lie in spurious local minima *during training* in the Kawaguchi model in the NTK regime.

#### Analysis in the initial state.

**Theorem 1** For any training pattern  $i$ , any output neuron  $j$ , and any path  $p$  from an input neuron to the output neuron  $j$  in the initial state immediately after the parameter initialization of the Kawaguchi model in the NTK regime,

$$P([Z_i]_{(j,p)} = 1) = \frac{1}{2^H} \quad (6)$$

where  $H$  is the number of hidden layers ( $H \geq 1$ ).  $\square$

*Proof.* Denote by  $j_1, \dots, j_H$  the hidden neurons on path  $p$  where  $j_k$  is the hidden neuron in the  $k$ -th hidden layer ( $k = 1, \dots, H$ ) (Fig. 3). Then,

$$\begin{aligned} P([Z_i]_{(j,p)} = 1) &= P(\text{Net input to the hidden neuron } j_k > 0 \ (k = 1, \dots, H)) \\ &= P(\mathbf{X}_i^T \mathbf{w}_{j_1} > 0, [\varphi(U_1^{(1)}) \cdots \varphi(U_{d_1}^{(1)})] \mathbf{w}_{j_2} > 0, \\ &\quad \cdots, [\varphi(U_1^{(H-1)}) \cdots \varphi(U_{d_{H-1}}^{(H-1)})] \mathbf{w}_{j_H} > 0) \end{aligned} \quad (7)$$

where  $\mathbf{X}_i \in I^{d_x}$  is the  $i$ -th input training pattern,  $\mathbf{w}_{j_k} \in \mathbb{R}^{d_{k-1}}$  is the weight vector of the hidden neuron  $j_k$  in the hidden layer  $k$ , and  $U_l^{(k)}$  is the net input to the hidden neuron  $l$  in the hidden layer  $k$  (Fig. 4).

We prove by mathematical induction that Eq. (6) holds true.

[For  $H = 1$ ] This case corresponds to a three-layered neural network. It follows that

$$\begin{aligned} P\left([Z_i]_{(j,p)} = 1\right) &= P(\mathbf{X}_i^T \mathbf{w}_{j_1} > 0) \quad (\text{from Eq.(7)}) \\ &= \frac{1}{2} \end{aligned} \quad (8)$$

where  $j_1$  is a hidden neuron on path  $p$ . We can see below that the last equality of Eq. (8) holds true. For a given input training pattern  $\mathbf{X}_i \in I^{d_x}$ ,  $\{\mathbf{w}_{j_1} \in \mathbb{R}^{d_x} \mid \mathbf{X}_i^T \mathbf{w}_{j_1} > 0\}$  is a half-open hyper-space with a normal vector  $\mathbf{X}_i$  through the origin in a  $d_x$ -dimensional Euclidean space (Fig. 5). According to the assumption, the random variables  $w_{j_1 1}, \dots, w_{j_1 d_x}$  which are the components of the weight vector  $\mathbf{w}_{j_1} = (w_{j_1 1} \dots w_{j_1 d_x})^T$  of the hidden neuron  $j_1$  obey the normal distribution  $(N, \sigma_x^2)$  independently. Consequently,  $P(\mathbf{X}_i^T \mathbf{w}_{j_1} > 0) = P(\mathbf{X}_i^T \mathbf{w}_{j_1} \leq 0)$ , which means  $P(\mathbf{X}_i^T \mathbf{w}_{j_1} > 0) = 1/2$ .

[For  $H$ ] This case corresponding to a deep ReLU neural network with  $H$  hidden layers, we show that if the case of  $H - 1$  holds, then case  $H$  also holds. Assuming that the case of  $H - 1$  holds, then

$$\begin{aligned} &P\left([Z_i]_{(j,p)} = 1\right) \\ &= P\left(\mathbf{X}_i^T \mathbf{w}_{j_1} > 0, \left[\varphi(U_1^{(1)}) \dots \varphi(U_{d_1}^{(1)})\right] \mathbf{w}_{j_2} > 0, \right. \\ &\quad \left. \dots, \left[\varphi(U_1^{(H-1)}) \dots \varphi(U_{d_{H-1}}^{(H-1)})\right] \mathbf{w}_{j_H} > 0\right) \quad (\text{Eq.(7) itself}) \\ &= P\left(\left[\varphi(U_1^{(1)}) \dots \varphi(U_{d_1}^{(1)})\right] \mathbf{w}_{j_2} > 0, \dots, \left[\varphi(U_1^{(H-1)}) \dots \varphi(U_{d_{H-1}}^{(H-1)})\right] \mathbf{w}_{j_H} > 0\right. \\ &\quad \left. \mid \mathbf{X}_i^T \mathbf{w}_{j_1} > 0\right) \cdot P\left(\mathbf{X}_i^T \mathbf{w}_{j_1} > 0\right). \end{aligned} \quad (9)$$

Here, the first factor of the right-hand-side of Eq. (9) represents the probability that the path passing through the  $H - 1$  hidden neurons  $j_2, \dots, j_H$  for the input training pattern  $[\varphi(U_1^{(1)}) \dots \varphi(U_{d_1}^{(1)})]^T \in \mathbb{R}^{d_1}$  such that  $U_{j_1}^{(1)} = \mathbf{X}_i^T \mathbf{w}_{j_1} > 0$  is active. Also, for any  $1 \leq s \leq d_1$ , by denoting  $\mathbf{X}_i = (x_1 \dots x_{d_0})^T$  and  $\mathbf{w}_s = (w_1 \dots w_{d_0})$  for the sake of simplicity,  $P(|\varphi(U_s^{(1)})| \leq |U_s^{(1)}| = |\mathbf{X}_i^T \mathbf{w}_s| \leq \alpha \sum_{t=1}^{d_0} |w_t| \leq 3\alpha d_0 \sigma_0 = \alpha) = 0.9973 \approx 1.0$  because each weight  $w_t$  obeys the normal distribution  $N(0, \sigma_0^2)$  where  $\sigma_0 = 1/(3d_0)$  which means  $P(|w_t| \leq 3\sigma_0 = 1/d_0) = 0.9973$  (the so-called three-sigma rule of thumb). Hence, according to the assumption of mathematical induction, the first factor of the right-hand-side of Eq. (9) is equal to  $(1/2)^{H-1}$ . In addition, the second factor of the right-hand-side of Eq. (9) is equal to  $1/2$  from Eq.(8). Therefore,

$$P\left([Z_i]_{(j,p)} = 1\right) = \left(\frac{1}{2}\right)^{H-1} \cdot \frac{1}{2}$$

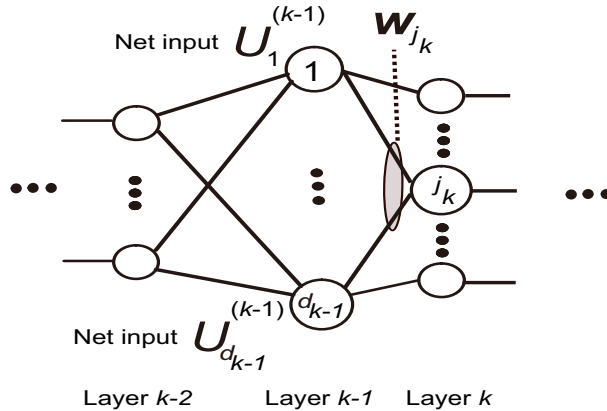


Figure 4: Relationship between the weight vector  $\mathbf{w}_{j_k}$  and the net inputs  $U_1^{(k-1)}, \dots, U_{d_{k-1}}^{(k-1)}$ .

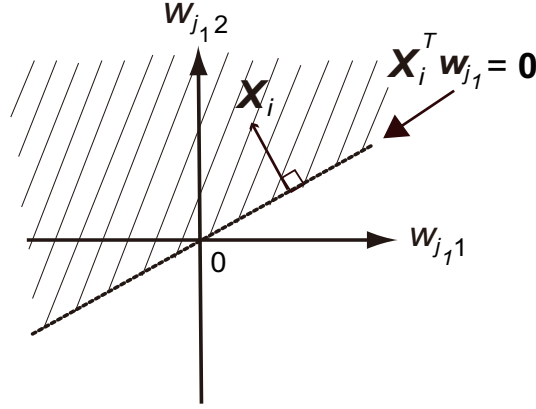


Figure 5: A half-open hyperspace  $\{\mathbf{w}_{j_1} = (w_{j_1,1} \ w_{j_1,2})^T \in \mathbb{R}^{d_x} \mid \mathbf{X}_i^T \mathbf{w}_{j_1} > 0\}$  (a half-open plane because  $d_x = 2$ ).

$$= \frac{1}{2^H}, \quad (10)$$

which means that the case of  $H$  indeed holds. Therefore, by mathematical induction, Eq. (6) holds for any  $H \geq 1$ . ■

Theorem 1 states that assumption A1p-m holds:  $\rho = 1/2^H$  in this case. Because

$$\begin{aligned} \lim_{H \rightarrow +\infty} P([Z_i]_{(j,p)} = 1) &= \lim_{H \rightarrow +\infty} \frac{1}{2^H} \\ &= 0, \end{aligned} \quad (11)$$

the probability that path  $p$  is active decreases exponentially. It converges to zero as the number of hidden layers  $H$  increases. The probability that path  $p$  is active decreases by half when a hidden layer is added.

**Theorem 2** *For any training pattern  $i$ , any output neuron  $j$ , and any path  $p$  from an input neuron to the output neuron  $j$  in the initial state immediately after the parameter initialization of the Kawaguchi model in the NTK regime, random variable  $[Z_i]_{(j,p)}$  is independent of the sequence of weights on path  $p$ .* □

At first glance, Theorem 2 seems counterintuitive because the random variable  $[Z_i]_{(j,p)}$  is a function of the sequence of weights on path  $p$  in the model with the finite widths of the hidden layers. However, Theorem 2 holds true because we deal with the deep ReLU neural network in the almost infinite-width limit. Actually, in the almost infinite-width limit, the absolute value of the product of an input value and the weight value on the path is negligibly small (see Eq. (13) in the supplementary material for details).

The reason why the next theorem 3 holds true is also as described above.

**Theorem 3** *For any training pattern  $i$ , any output neuron  $j$ , and any path  $p$  from an input neuron to the output neuron  $j$  in the initial state immediately after the parameter initialization of the Kawaguchi model in the NTK regime, random variable  $[Z_i]_{(j,p)}$  is independent of the input training signal  $\mathbf{X}_i$ .* □

The proofs of Theorem 2 and Theorem 3 are in the supplementary material.

Theorem 2 and Theorem 3 state that assumption A5u-m-1 holds in the initial state immediately after the parameter initialization of the Kawaguchi model in the NTK regime.

Thus, it follows from Theorems 1-3 that assumptions A1p-m and A5u-m (A5u-m-1) hold in the initial state immediately after the parameter initialization of the Kawaguchi model in the NTK regime, both of which were introduced in [15]. Therefore, the error function  $L(\Theta)$  does not lie in spurious local minima in the initial state immediately after the parameter initialization under the NTK regime according to Corollary 1. Therefore, we obtain the following theorem.

**Theorem 4** Let  $q = \rho^{-1} = 2^H$ . Assume that  $\mathbf{X}\mathbf{X}^T$  and  $\mathbf{X}\mathbf{Y}^T$  are full rank. Then, the error function  $L(\Theta)$  does not lie in spurious local minima in the initial state of the Kawaguchi model in the NTK regime immediately after the parameter initialization.  $\square$

**Analysis during training.** Next, we make clear spurious local minima *during training* of the Kawaguchi model in the NTK regime. Jacot et al. theoretically proved that the behavior of neural networks during training is described by a related kernel called the neural tangent kernel (NTK) in the limit as the widths of the hidden layers tend to infinity [21]: let  $f_{\theta(t)}$  be the network function of a neural network which maps an input vector to an output vector where  $\theta(t)$  is the vector of the parameters of the neural network after the  $t$ -th learning; then, during gradient descent, the dynamics of the network function  $f_{\theta(t)}$  follows that of the so-called kernel gradient descent in function space with respect to a limiting kernel, which only depends on the depth of the network, the choice of nonlinearity and the initialization variance. More specifically, they proved that for a least-squares regression cost, if  $f_{\theta(0)}$  is initialized with a normal distribution, then the infinite-width limit network function  $f_{\theta(t)}$  has the normal distribution for all times  $t$ , and in particular at convergence  $t \rightarrow \infty$ . They also made numerical experiments on a ReLU deep neural network with a least-squares cost and confirmed that the distributions of the network functions are very similar for both widths of 50 and 1000: their mean and variance after the 1000th learning appear to be close to those of the limiting distribution  $t \rightarrow \infty$ .

Several researchers also proved that the parameters of deep nonlinear neural networks move little from their initial values during training such as the stochastic gradient descent in the NTK regime [22–24]. Especially, Allen-Zhu et al. proved it for deep ReLU neural networks [22]. Therefore, we realize that the parameters always has the same normal distribution as the initial state during training of the Kawaguchi model in the NTK regime.

As a consequence, from Theorem 4, we obtain the following theorem.

**Theorem 5** Let  $q = \rho^{-1} = 2^H$ . Assume that  $\mathbf{X}\mathbf{X}^T$  and  $\mathbf{X}\mathbf{Y}^T$  are full rank. Then, the error function  $L(\Theta)$  does not lie in spurious local minima during training of the Kawaguchi model in the NTK regime.  $\square$

### 3 Discussion

He et al. proposed a weight initialization method for neural networks with the ReLU activation function which is commonly used in practice: the initial value of each weight between the layer  $i$  and the layer  $i + 1$  is set according to either of the normal distributions  $N(0, 2/n_i)$  or  $N(0, 2/n_{i+1})$  independently where  $n_i$  is the number of neurons in the layer  $i$  [26]. This was derived by keeping the variance of the net input vector in each layer equal and keeping the variance of the back-propagated gradients equal, respectively, for the purpose of avoiding their saturation. Thus, the learning dynamics of the deep ReLU neural networks where the widths of the hidden layers are sufficiently large and the parameters are initialized by the He initialization method belongs to the NTK regime. Therefore, the error function does not lie in spurious local minima in the loss landscape of the Kawaguchi model initialized by the He method during training in the NTK regime.

Lee et al. theoretically showed that the learning dynamics with a certain learning rate in parameter space of deep nonlinear neural networks are exactly described by a linearized model where the parameters of the deep neural networks move little from their initial values in the NTK regime [24]. They did not address the property on local minima in the NTK regime. In contrast, we addressed it in this paper and obtained the result that the deep ReLU neural networks do not lie in spurious local minima during training under the NTK regime. Thus, the result in [24] and the one of this paper are complementary.

### 4 Conclusions

We theoretically proved that the deep ReLU neural networks do not lie in spurious local minima in the loss landscape under the Neural Tangent Kernel (NTK) regime, that is, in the gradient descent training dynamics of the deep ReLU neural networks whose parameters are initialized by a normal distribution in the limit as the widths of the hidden layers tend to infinity. Especially, the error function does not lie in spurious local minima in the loss landscape of the Kawaguchi model



initialized by the He initialization method which is commonly used in practice during training in the NTK regime. The results obtained in this paper approximately hold true for a family of ReLU activation functions such as the softplus activation function  $f(x) = \log(1 + \exp(x))$  [27]. In future studies, we will make clear the property of the local minima of deep nonlinear neural networks with the activation functions except the ReLU function in the NTK regime.

## Acknowledgments

The author would like to give special thanks to Dr. R. Karakida, AIST, for his valuable comments. This work was supported by JSPS KAKENHI Grant Number JP16K00347.

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## Supplementary material: Spurious Local Minima of Deep ReLU Neural Networks in the Neural Tangent Kernel Regime

**Proof of Theorem 2.** Take training pattern  $i$ , output neuron  $j$ , and path  $p$  from an input neuron to output neuron  $j$  of the Kawaguchi model in the NTK regime arbitrarily and fix them. Denote by  $j_0, \dots, j_H$  the neurons on path  $p$  where  $j_k$  is the neuron in the  $k$ -th layer ( $k = 0, \dots, H$ ). Let also  $w_{j_1 j_0}, \dots, w_{j_{H+1} j_H}$  denote  $H + 1$  weights on path  $p$  where  $w_{j_{k+1} j_k}$  is the weight between the layer  $k$  and the layer  $k + 1$  on path  $p$  ( $k = 0, \dots, H$ ) (Fig. 6). Then, for any  $\lambda_1, \dots, \lambda_{H+1} \in \mathbb{R}$ ,

$$\begin{aligned}
& P \left( [Z_i]_{(j,p)} = 1 \mid w_{j_1 j_0} = \lambda_1, \dots, w_{j_{H+1} j_H} = \lambda_{H+1} \right) \\
&= P \left( \mathbf{X}_i^T \mathbf{w}_{j_1} > 0, \left[ \varphi(U_1^{(1)}) \cdots \varphi(U_{d_1}^{(1)}) \right] \mathbf{w}_{j_2} > 0, \dots, \left[ \varphi(U_1^{(H-1)}) \cdots \varphi(U_{d_{H-1}}^{(H-1)}) \right] \mathbf{w}_{j_H} > 0 \right. \\
&\quad \left. \mid w_{j_1 j_0} = \lambda_1, \dots, w_{j_H j_{H-1}} = \lambda_H \right) \quad (\text{from Eq.(7)}) \\
&\quad (w_{j_{H+1} j_H} = \lambda_{H+1} \text{ is removed because it is independent of } [Z_i]_{(j,p)}) \\
&\stackrel{=}{=} \frac{1}{2^H}. \tag{12}
\end{aligned}$$

Here, we can regard that  $\lambda_k$  satisfies the inequality  $|\lambda_k| \leq 3\sigma_{k-1} = 1/d_{k-1}$  ( $k = 1, \dots, H + 1$ ) because the weight  $w_{j_k j_{k-1}}$  obeys the normal distribution  $N(0, \sigma_{k-1}^2)$  where  $\sigma_{k-1} = 1/(3d_{k-1})$  which means  $P(|w_{j_k j_{k-1}}| \leq 3\sigma_{k-1} = 1/d_{k-1}) = 0.9973$  (the so-called three-sigma rule of thumb).

We prove below by mathematical induction that the approximate equality ( $\stackrel{=}{=}$ ) in Eq. (12) holds true.

[For  $H = 1$ ] This case corresponds to a three-layered neural network. For the sake of simplicity, we let  $\mathbf{X}_i = (x_1 \cdots x_{j_0} \cdots x_{d_0})^T$  and  $\mathbf{w}_{j_1} = (w_1 \cdots w_{j_0} \cdots w_{d_0})^T$  where  $w_{j_0} = w_{j_1 j_0}$ . Then,

$$P \left( \mathbf{X}_i^T \mathbf{w}_{j_1} > 0 \mid w_{j_1 j_0} = \lambda_1 \right)$$

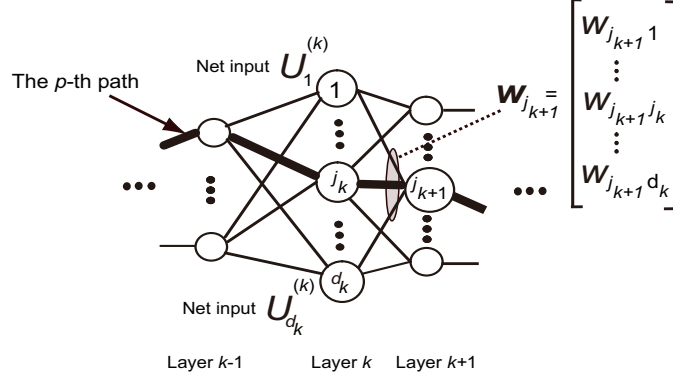


Figure 6: Relationship between the weight vector  $w_{j_{k+1}}$  and the net inputs  $U_1^{(k)}, \dots, U_{d_k}^{(k)}$  in Eq. (12).

$$\begin{aligned}
&= P\left(x_1 w_1 + \dots + x_{j_0} w_{j_1 j_0} + \dots + x_{d_0} w_{d_0} > 0 \mid w_{j_1 j_0} = \lambda_1\right) \\
&= P\left(x_1 w_1 + \dots + x_{j_0} \lambda_1 + \dots + x_{d_0} w_{d_0} > 0 \mid w_{j_1 j_0} = \lambda_1\right) \\
&= P\left(x_1 w_1 + \dots + x_{j_0} \lambda_1 + \dots + x_{d_0} w_{d_0} > 0\right) \\
&\quad (w_{j_1 j_0} = \lambda_1 \text{ is removed because it is independent of the other weights}) \\
&= P\left(x_1 w_1 + \dots + x_{j_0-1} w_{j_0-1} + x_{j_0+1} w_{j_0+1} + \dots + x_{d_0} w_{d_0} > -x_{j_0} \lambda_1\right) \\
&\doteq P\left(x_1 w_1 + \dots + x_{j_0-1} w_{j_0-1} + x_{j_0+1} w_{j_0+1} + \dots + x_{d_0} w_{d_0} > 0\right) \tag{13} \\
&\quad (\text{because } |x_{j_0} \lambda_1| \leq 3\alpha\sigma_0 = \alpha/d_0 \text{ and the number of input neurons } d_0 \text{ is sufficiently large}) \\
&= \frac{1}{2}. \quad (\text{for the same reason that the last equality of Eq. (8) holds true.}) \tag{14}
\end{aligned}$$

[For  $H$ ] This case corresponding to a deep ReLU neural network with  $H$  hidden layers, we show that if the case of  $H-1$  holds, then case  $H$  also holds. Assuming that the case of  $H-1$  holds, then

$$\begin{aligned}
&P\left(\mathbf{X}_i^T \mathbf{w}_{j_1} > 0, \left[\varphi(U_1^{(1)}) \dots \varphi(U_{d_1}^{(1)})\right] \mathbf{w}_{j_2} > 0, \dots, \left[\varphi(U_1^{(H-1)}) \dots \varphi(U_{d_{H-1}}^{(H-1)})\right] \mathbf{w}_{j_H} > 0 \right. \\
&\quad \left. \mid w_{j_1 j_0} = \lambda_1, \dots, w_{j_H j_{H-1}} = \lambda_H\right) \\
&= P\left(\left[\varphi(U_1^{(1)}) \dots \varphi(U_{d_1}^{(1)})\right] \mathbf{w}_{j_2} > 0, \dots, \left[\varphi(U_1^{(H-1)}) \dots \varphi(U_{d_{H-1}}^{(H-1)})\right] \mathbf{w}_{j_H} > 0 \right. \\
&\quad \left. \mid \mathbf{X}_i^T \mathbf{w}_{j_1} > 0, w_{j_1 j_0} = \lambda_1, \dots, w_{j_H j_{H-1}} = \lambda_H\right) \cdot \\
&\quad P\left(\mathbf{X}_i^T \mathbf{w}_{j_1} > 0 \mid w_{j_1 j_0} = \lambda_1, \dots, w_{j_H j_{H-1}} = \lambda_H\right) \\
&= P\left(\left[\varphi(U_1^{(1)}) \dots \varphi(U_{d_1}^{(1)})\right] \mathbf{w}_{j_2} > 0, \dots, \left[\varphi(U_1^{(H-1)}) \dots \varphi(U_{d_{H-1}}^{(H-1)})\right] \mathbf{w}_{j_H} > 0 \right. \\
&\quad \left. \mid \mathbf{X}_i^T \mathbf{w}_{j_1} > 0, w_{j_1 j_0} = \lambda_1, \dots, w_{j_H j_{H-1}} = \lambda_H\right) \cdot P\left(\mathbf{X}_i^T \mathbf{w}_{j_1} > 0 \mid w_{j_1 j_0} = \lambda_1\right). \tag{15} \\
&\quad (w_{j_2 j_1} = \lambda_2, \dots, w_{j_H j_{H-1}} = \lambda_H \text{ are removed because they are independent of } \mathbf{w}_{j_1})
\end{aligned}$$

Here, the first factor of the right-hand-side of Eq. (15) represents the probability that the path passing through the  $H-1$  hidden neurons  $j_2, \dots, j_H$  for the input training pattern  $[\varphi(U_1^{(1)}) \dots \varphi(U_{d_1}^{(1)})]^T \in \mathbb{R}^{d_1}$  such that  $U_{j_1}^{(1)} = \mathbf{X}_i^T \mathbf{w}_{j_1} > 0$  and  $w_{j_1 j_0} = \lambda_1$  is active. Also, for any  $1 \leq s \leq d_1$ , by denoting  $\mathbf{X}_i = (x_1 \dots x_{d_0})^T$  and  $\mathbf{w}_s = (w_1 \dots w_{d_0})$  for the sake of simplicity,  $P(|\varphi(U_s^{(1)})| \leq |U_s^{(1)}|) = |\mathbf{X}_i^T \mathbf{w}_s| \leq \alpha \sum_{t=1}^{d_0} |w_t| \leq 3\alpha d_0 \sigma_0 = \alpha = 0.9973 \doteq 1.0$  because each weight  $w_t$  obeys the normal distribution  $N(0, \sigma^2/d_0)$  which means  $P(|w_t| \leq 3\sigma_0 = 1/d_0) = 0.9973$  (the so-called three-sigma rule of thumb). Hence, according to the assumption of mathematical induction, the first

factor of the right-hand-side of Eq. (15) is nearly equal to  $(1/2)^{H-1}$ . In addition, the second factor of the right-hand-side of Eq. (15) is nearly equal to  $1/2$  from Eq.(14). So,

$$\begin{aligned}
& P \left( \mathbf{X}_i^T \mathbf{w}_{j_1} > 0, \left[ \varphi(U_1^{(1)}) \cdots \varphi(U_{d_1}^{(1)}) \right] \mathbf{w}_{j_2} > 0, \dots, \left[ \varphi(U_1^{(H-1)}) \cdots \varphi(U_{d_{H-1}}^{(H-1)}) \right] \mathbf{w}_{j_H} > 0 \right. \\
& \qquad \qquad \qquad \left. \left| w_{j_1 j_0} = \lambda_1, \dots, w_{j_H j_{H-1}} = \lambda_H \right) \right. \\
& \doteq \left( \frac{1}{2} \right)^{H-1} \cdot \frac{1}{2} \\
& = \frac{1}{2^H}, \tag{16}
\end{aligned}$$

which means that the case of  $H$  indeed holds. Thus, by mathematical induction, Eq. (12) holds for any  $H \geq 1$ . Therefore,

$$\begin{aligned}
& P \left( [Z_i]_{(j,p)} = 1 \mid w_{j_1 j_0} = \lambda_1, \dots, w_{j_{H+1} j_H} = \lambda_{H+1} \right) \\
& \doteq \frac{1}{2^H} \quad (\text{from Eq. (12)}) \\
& = P \left( [Z_i]_{(j,p)} = 1 \right). \quad (\text{from Theorem 1}) \tag{17}
\end{aligned}$$

This completes the proof. ■

**Proof of Theorem 3** . Take training pattern  $i$ , output neuron  $j$ , path  $p$  from an input neuron to output neuron  $j$  of the deep ReLU neural network in the Kawaguchi model in the NTK regime initialized by the normal distribution  $N(0, \sigma_l^2)$  where  $\sigma_l = 1/(3d_l)$  and  $d_l$  is the number of neurons in the layer  $l$ , and  $\boldsymbol{\mu} \in \mathbb{R}^{d_x}$  arbitrarily and fix them. Then, in the same mode of the proof of Theorem 1, it is apparent that

$$P \left( [Z_i]_{(j,p)} = 1 \mid \mathbf{X}_i = \boldsymbol{\mu} \right) = \frac{1}{2^H}. \tag{18}$$

Therefore, it follows that

$$\begin{aligned}
P \left( [Z_i]_{(j,p)} = 1 \right) & = \frac{1}{2^H} \quad (\text{from Theorem1}) \\
& = P \left( [Z_i]_{(j,p)} = 1 \mid \mathbf{X}_i = \boldsymbol{\mu} \right) \quad (\text{from Eq.(18)}) \tag{19}
\end{aligned}$$

holds true. Eq. (19) completes the proof. ■