

Neural Networks

Neural Networks 13 (2000) 317-327

www.elsevier.com/locate/neunet

Contributed article

# Local minima and plateaus in hierarchical structures of multilayer perceptrons

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Received 6 May 1999; received in revised form 14 December 1999; accepted 14 December 1999

## Abstract

Local minima and plateaus pose a serious problem in learning of neural networks. We investigate the hierarchical geometric structure of the parameter space of three-layer perceptrons in order to show the existence of local minima and plateaus. It is proved that a critical point of the model with H - 1 hidden units always gives many critical points of the model with H hidden units. These critical points consist of many lines in the parameter space, which can cause plateaus in learning of neural networks. Based on this result, we prove that a point in the critical lines corresponding to the global minimum of the smaller model can be a local minimum or a saddle point of the larger model. We give a necessary and sufficient condition for this, and show that this kind of local minimum exist as a line segment if any. The results are universal in the sense that they do not require special properties of the target, loss functions and activation functions, but only use the hierarchical structure of the model. © 2000 Elsevier Science Ltd. All rights reserved.

Keywords: Multilayer perceptron; Local minima; Plateau; Error surface

## 1. Introduction

It has been believed that the error surface of multilayer perceptrons (MLP) has in general many local minima. This has been regarded as one of the disadvantages of neural networks, and a great deal of effort has been paid to find good methods of avoiding them and achieving the global minimum.

There have been no rigorous results, however, to prove the existence of local minima. Even in the simple example of the XOR problem, existence of local minima had been a controversial problem. Lisboa and Perantonis (1991) elucidated all the critical points of the XOR problem and asserted with a help of numerical simulations that some of them are local minima. Recently, Hamney (1998) and Sprinkhuizen-Kuyper and Boers (1998a,b) rigorously proved that what have been believed to be local minima in Lisboa and Perantonis (1991) correspond to local minima with infinite parameter values, and that there always exists a strictly decreasing path from each finite point to the global minimum. Thus, there are no local minima in the finite weight region for the XOR problem. Existence of local minima in general cases has been an open problem in the rigorous mathematical sense.

It is also difficult to derive meaningful results on local minima from numerical experiments. In practical applications, we often see extremely slow dynamics around a point that differs from the global minimum. However, it is not easy to tell rigorously whether it is a local minimum. It is known that a typical learning curve shows a *plateau* in the middle of training, which causes very slow decrease of the training error for a long time before a sudden exit from it (Amari, 1998; Saad & Solla, 1995). A plateau can be easily misunderstood as a local minimum in practical problems.

This paper discusses critical points of the MLP model, which are caused by the hierarchical structure of the models having a smaller number of hidden units. For simplicity, we discuss only the MLP model with a one-dimensional output in this paper. The input-output function space of networks with H - 1 hidden units is included in the function space of networks with H hidden units. However, the relation between the parameter spaces of these two models is not so simple (see Chen, Lu & Hecht-Nielsen, 1993; Rüger & Ossen, 1997). Sussmann (1992) elucidated the condition that a function described by a network with H hidden units can be realized by a network with H - 1 hidden units in the case of activation function. In this paper, we further investigate the geometric structure of the parameters

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of networks which are realizable by a network with H - 1hidden units. In particular, we elucidate how they can be embedded in the parameter space of H hidden units. Based on the geometric structure, we show that a critical point of the error surface for the MLP model with H - 1 hidden units gives a set of critical points in the parametric space of the MLP with *H* hidden units.

The main purpose of the present paper is to show that a subset of critical points corresponding to the global minimum of a smaller network can be local minima or saddles of the larger network. More precisely, the subset of critical points on which the input-output behavior is the same is divided into two parts, one consisting of local minima and the other saddle points. We give an explicit condition when this occurs. This gives a formal proof of the existence of local minima for the first time. Moreover, the coexistence of local minima and saddles in one equivalent set of critical points explains a serious mechanism of plateaus: when such is the case the network parameters are attracted in the part of local minima, stay and walk randomly for a long time in that flat region on which the performance is the same, but eventually go out from the part of saddles in the region. This is a new type of critical points in nonlinear dynamics given rise to by the hierarchical structure of a model.

This paper is organized as follows. In Section 2, after showing the necessary definitions and terminologies, we elucidate the geometric or topological structure of the parameter space. Section 3 discusses critical points of the error surface. In Section 4, we mathematically prove the coexistence of local minima and saddles under one condition. This shows not only the existence of local minima but also a possible mechanism of plateaus. We also show the results of numerical simulations realizing local minima. Section 5 contains conclusion and discussion.

## 2. Geometric structure of the parameter space

#### 2.1. Basic definitions

In this paper, we consider a three-layer perceptron with one linear output unit and L input units. The input-output relation of a network with H hidden units is described by the function:

$$f^{(H)}(\mathbf{x}; \mathbf{\theta}^{(H)}) = \sum_{j=1}^{H} v_j \varphi(\mathbf{w}_j^{\mathrm{T}} \mathbf{x} + w_{j0}) + v_0, \qquad (1)$$

where T denotes transposition,  $\mathbf{x} = (x_1, ..., x_L)^T \in \mathbb{R}^L$  is an input vector,  $\mathbf{w}_j = (w_{j1}, ..., w_{jL})^T \in \mathbb{R}^L (1 \le j \le H)$  is the weight vector of the *j*th hidden unit and  $\mathbf{\theta}^{(H)} = (v_0, v_1, ..., v_H, w_{10}, \mathbf{w}_1^T, ..., w_{H0}, \mathbf{w}_H^T)^T$  summarizes all the parameters in one large vector. The function  $\varphi(t)$  is called an activation function. In this paper, we use tanh for  $\varphi$ . Introducing the

notations:

$$\tilde{\mathbf{x}} = \begin{pmatrix} 1 \\ \mathbf{x} \end{pmatrix} \in \mathbb{R}^{L+1}, \ \tilde{\mathbf{w}}_j = \begin{pmatrix} w_{j0} \\ \mathbf{w}_j \end{pmatrix} \in \mathbb{R}^{L+1}, \ (1 \le j \le H),$$
(2)

for simplicity, we can write

$$f^{(H)}(\mathbf{x}; \mathbf{\theta}^{(H)}) = \sum_{j=1}^{H} v_j \varphi(\tilde{\mathbf{w}}_j^{\mathrm{T}} \tilde{\mathbf{x}}) + v_0.$$
(3)

Using the result of Kůrkova and Kainen (1994), all the theorems obtained in this paper are applicable for other sigmoid- or bell-shaped activation functions with necessary modifications. We will show this later. We use the linear activation in the output layer. However, all the results are easily extended to a model with a monotone nonlinear output unit, because this causes only a nonlinear rescaling of the output data.

Given N input-output training data  $\{(\mathbf{x}^{(\nu)}, y^{(\nu)}) | \nu =$ 1, ..., N, we use a MLP model to realize the relation expressed by the data. The objective of training is to find the parameter that minimizes the error function defined by:

$$E_{H}(\mathbf{\theta}^{(H)}) = \sum_{\nu=1}^{N} \ell(y^{(\nu)}, f(\mathbf{x}^{(\nu)}; \mathbf{\theta}^{(H)})),$$
(4)

where  $\ell(y, z)$  is a loss function such that  $\ell(y, z) \ge 0$  and the equality holds if and only if y = z. When  $\ell(y, z) =$  $(1/2)||y - z||^2$ , the objective function is the mean square error. We can use other loss functions such as  $L_p$  norm  $\ell(y,z) = 1/p ||y-z||^p$  and the cross entropy  $\ell(y,z) =$  $-\sigma(y)\log \sigma(z) - (1 - \sigma(y))\log(1 - \sigma(z))$ , where  $\sigma(t)$  is a sigmoidal function for the nonlinearity of the output unit. The results in this paper are independent of the choice of a loss function.

## 2.2. Hierarchical structure of MLP

The parameter vector  $\mathbf{\theta}^{(H)}$  consists of a LH + 2H + 1dimensional Euclidean space  $\Theta_{H}$ . Each  $\mathbf{\theta}^{(H)}$  gives a nonlinear function Eq. (1) of  $\mathbf{x}$ , so that the set of all the functions realized by  $\Theta_H$  is a function space described by:

$$\mathscr{S}_{H} = \{ f^{(H)}(\mathbf{x}; \mathbf{\theta}^{(H)}) : \mathbb{R}^{L} \to \mathbb{R} | \mathbf{\theta}^{(H)} \in \mathcal{O}_{H} \}.$$
(5)

We denote the mapping from  $\Theta_H$  onto  $\mathscr{S}_H$  by

$$\pi_H: \mathcal{O}_H \to \mathscr{S}_H, \qquad \mathbf{\theta}^{(H)} \mapsto f(\mathbf{x}; \mathbf{\theta}^{(H)}).$$
 (6)

We sometimes write  $f_{\boldsymbol{\theta}}^{(H)}$  for  $\pi_{H}(\boldsymbol{\theta})$ . It is important to note that  $\pi_{H}$  is *not* one-to-one, that is, different  $\hat{\mathbf{\theta}}^{(H)}$  may give the same input–output function. The interchange between  $(v_{j_1}, \mathbf{w}_{j_1})$  and  $(v_{j_2}, \mathbf{w}_{j_2})$  does not alter the image of  $\pi_{H}$ . In the case of tanh activation function, Chen et al. (1993) showed that any analytic map  $T : \Theta_H \to \Theta_H$  such that  $f^{(H)}(\mathbf{x}; T(\mathbf{\theta}^{(H)})) = f^{(H)}(\mathbf{x}; \mathbf{\theta}^{(H)})$  is a composition of hidden unit weight interchanges and hidden unit weight sign flips, which later are defined by  $(v_i, \tilde{\mathbf{w}}_i) \mapsto (-v_i, -\tilde{\mathbf{w}}_i)$ .



Fig. 1. A network given by a parameter in  $\mathscr{A}_j$ ,  $\mathscr{B}_j$  and  $\mathscr{C}_{j_1 j_2}^{\pm}$ .

These transforms consist of an algebraic group  $G_H$ , which is isomorphic to a direct product of Weyl groups. We write  $T_g$ for the transform given by  $g \in G_H$ .

The function spaces  $\mathscr{G}_H$  (H = 0, 1, 2, ...) have a trivial hierarchical structure:

$$\mathcal{S}_0 \subset \mathcal{S}_1 \subset \cdots \subset \mathcal{S}_{H-1} \subset \mathcal{S}_H \subset \cdots.$$
(7)

The inclusion is denoted by  $\iota_{H-1} : \mathscr{G}_{H-1} \hookrightarrow \mathscr{G}_{H}$ . On the other hand, the parameter space of the smaller networks is not canonically included in  $\Theta_{H}$ . Given a function  $f_{\theta}^{(H-1)}$  realized by a network with H - 1 hidden units, there are a family of networks with H hidden units and parameters  $\theta^{(H)}$  that realizes the same function  $f_{\theta}^{(H-1)}$ . In other words, a map from  $\theta^{H-1}$  to  $\theta^{H}$  that commutes the following diagram is not unique.

The set of all the parameters  $\mathbf{\theta}^{(H)}$  that realize the input– output functions of networks with H - 1 hidden units is denoted by:

$$\Omega_H = \pi_H^{-1}(\iota_{H-1}(\mathscr{S}_{H-1})).$$
(9)

From Sussmann's result (Sussmann, 1992; Theorem 1 and its corollary), the parameter set  $\Omega_H$  is the union of the following submanifolds of  $\Theta_H$  (see Fig. 1):

$$\mathscr{A}_j = \{ \mathbf{\theta}^{(H)} \in \mathcal{O}_H | v_j = 0 \} \qquad (1 \le j \le H), \tag{10}$$

$$\mathscr{B}_j = \{ \mathbf{0}^{(H)} \in \mathcal{O}_H | \mathbf{w}_j = \mathbf{0} \} \qquad (1 \le j \le H), \tag{11}$$

$$\mathscr{C}_{j_1 j_2}^{\pm} = \{ \boldsymbol{\theta}^{(H)} \in \boldsymbol{\Theta}_H | \tilde{\mathbf{w}}_{j_1} = \pm \tilde{\mathbf{w}}_{j_2} \} \qquad (1 \le j_1 < j_2 \le H).$$
(12)

Here,  $\mathscr{A}_j$  is the set of parameters where  $v_j = 0$  so that the *j*th hidden units plays no role. Similarly, the *j*th hidden unit has 0 weight in  $\mathscr{B}_j$  so that it outputs only a constant bias term. In  $\mathscr{C}_{j_1j_2}^{\pm}$ , the *j*<sub>1</sub>th hidden unit and *j*<sub>2</sub>th hidden unit have the same (or opposite) weight vector and bias, so that their behaviors are the same (opposite). They may be integrated into one

unit, where  $v_1 \pm v_2$  is the weight of the new unit to the output unit. From the viewpoint of mathematical statistics, it is also proved by Fukumizu (1996) that  $\Omega$  is the set of all the points at which the Fisher information matrix is singular.

We further investigate how each function in  $\mathscr{S}_{H-1}$  is. Let  $f_{\boldsymbol{\theta}^{(H-1)}}^{(H-1)}$  be a function in  $\mathscr{S}_{H-1}$ - $\mathscr{S}_{H-2}$ . To distinguish  $\boldsymbol{\Theta}_{H-1}$  from  $\boldsymbol{\Theta}_{H}$ , we use different parameter variables and indexing:

$$f^{(H-1)}(\mathbf{x}; \mathbf{\theta}^{(H-1)}) = \sum_{j=2}^{H} \zeta_j \varphi(\tilde{\mathbf{u}}_j^{\mathrm{T}} \tilde{\mathbf{x}}) + \zeta_0.$$
(13)

Let  $\Omega_H(\mathbf{0}^{(H-1)})$  be the set of parameters  $\mathbf{0}^{(H)}$  that realizes a given  $f_{\mathbf{0}^{(H-1)}}^{(H-1)}$ ;

$$\Omega_{H}(\mathbf{\theta}^{(H-1)}) = \pi_{H}^{-1}(\iota_{H-1}(f_{\mathbf{\theta}^{(H-1)}}^{(H-1)}).$$
(14)

Then,  $\Omega_H(\mathbf{\theta}^{(H-1)})$  is the union of the submanifolds in each of  $\mathscr{A}_j$ ,  $\mathscr{B}_j$  and  $\mathscr{C}_{j_1 j_2}^{\pm}$ . For simplicity, we show only an example of the submanifolds of  $\mathscr{A}_1$ ,  $\mathscr{B}_1$  and  $\mathscr{C}_{12}^+$ ;

$$\begin{split} \mathbf{\Lambda} &= \{ \mathbf{\theta}^{(H)} \in \mathcal{O}_H | v_1 = 0, v_0 = \zeta_0, v_j = \zeta_j, \, \tilde{\mathbf{w}}_j = \tilde{\mathbf{u}}_j, \\ (2 \le j \le H) \} \\ \Xi &= \{ \mathbf{\theta}^{(H)} \in \mathcal{O}_H | \mathbf{w}_1 = \mathbf{0}, v_1 \varphi(w_{10}) + v_0 = \zeta_0, v_j = \zeta_j, \, \tilde{\mathbf{w}}_j = \tilde{\mathbf{u}}_j, \end{split}$$

$$(2 \le j \le H)\}$$

$$\Gamma = \{ \mathbf{\Theta}^{(H)} \in \Theta_H | \tilde{\mathbf{w}}_1 = \tilde{\mathbf{w}}_2 = \tilde{\mathbf{u}}_2, v_0 = \zeta_0, v_1 + v_2 = \zeta_2, v_j = \zeta_j, v_j = \zeta_j \}$$

$$\tilde{\mathbf{w}}_j = \tilde{\mathbf{u}}_j, (3 \le j \le H)\}.$$
(15)

The submanifold  $\Lambda$  is an L + 1 dimensional affine space parallel to the  $\tilde{\mathbf{w}}_1$ -plane because  $\tilde{\mathbf{w}}_1$  may take arbitrary values in it, but all the other components of  $\boldsymbol{\theta}^{(H)}$  are determined by prescribed  $\boldsymbol{\theta}^{(H-1)}$ . The set  $\Xi$  is a two-dimensional submanifold defined by a nonlinear equation:

$$v_1 \varphi(w_{10}) + v_0 = \zeta_0, \tag{16}$$

where  $v_0$ ,  $v_1$  and  $w_{10}$  can take arbitrary values provided they satisfy the above. The  $\Gamma$  set is a line in the  $v_1v_2$ -plane, defined by  $v_1 + v_2 = \zeta_2$ . It is known that all the other components in  $\Omega(\mathbf{0}^{(H-1)})$  are obtained as the transforms of  $\Lambda$ ,  $\Xi$  and  $\Gamma$  by  $g \in G_H$  (Kůrkova & Kainen, 1994; Sussmann, 1992). For example, the image of  $\Gamma$  by the



Fig. 2. Embedding  $\alpha_{\tilde{w}}$ 

sign flip about the second hidden unit is given by:

$$\Gamma^{(-1)} = \{ \mathbf{\theta}^{(H)} \in \Theta_H | \tilde{\mathbf{w}}_1 = -\tilde{\mathbf{w}}_2 = \tilde{\mathbf{u}}_2, v_0 = \zeta_0, v_1 - v_2 = \zeta_2, v_j = \zeta_j, \tilde{\mathbf{w}}_j = \tilde{\mathbf{u}}_j, (3 \le j \le H) \}.$$
(17)

The image of  $\Lambda$ ,  $\Xi$  and  $\Gamma$  by a hidden-unit interchange is trivial. Thus, each function of a smaller network is realized not by discrete points but by high-dimensional submanifolds in  $\Omega_{H}$ .

In order to make analysis more concrete, we give a definite correspondence between  $\Theta_{H-1}$  and  $\Theta_H$  that realize the same function. We define the following canonical embeddings of  $\Theta_{H-1}$  into  $\Theta_H$ , which commute the diagram (8), using  $\tilde{\mathbf{w}} \in \mathbb{R}^{L+1}$ ,  $(v, w) \in \mathbb{R}^2$  and  $\lambda \in \mathbb{R}$  as their parameters.

$$\begin{split} \alpha_{\tilde{\mathbf{w}}} &: \mathcal{O}_{H-1} \to \mathcal{O}_{H}, \ \mathbf{\theta}^{(H-1)} \mapsto (\zeta_{0}, 0, \zeta_{2}, ..., \zeta_{H}, \tilde{\mathbf{w}}^{\mathrm{T}}, \tilde{\mathbf{u}}_{2}^{\mathrm{T}}, ..., \tilde{\mathbf{u}}_{H}^{\mathrm{T}})^{\mathrm{T}}, \\ \beta_{(v,w)} &: \mathcal{O}_{H-1} \to \mathcal{O}_{H}, \ \mathbf{\theta}^{(H-1)} \mapsto (\zeta_{0} - v\varphi(w), v, \zeta_{2}, ..., \zeta_{H}, \\ (w, \mathbf{0}^{\mathrm{T}}), \tilde{\mathbf{u}}_{2}^{\mathrm{T}}, ..., \tilde{\mathbf{u}}_{H}^{\mathrm{T}})^{\mathrm{T}}, \\ \gamma_{\lambda} &: \mathcal{O}_{H-1} \to \mathcal{O}_{H}, \\ \mathbf{\theta}^{(H-1)} \mapsto (\zeta_{0}, \lambda\zeta_{2}, (1-\lambda)\zeta_{2}, \zeta_{3}, ..., \zeta_{H}, \tilde{\mathbf{u}}_{2}^{\mathrm{T}}, \tilde{\mathbf{u}}_{3}^{\mathrm{T}}, ..., \tilde{\mathbf{u}}_{H}^{\mathrm{T}})^{\mathrm{T}}. \end{split}$$

These maps are illustrated in Figs. 2–4. If we change the parameter of each embedding, the images of  $\mathbf{\theta}^{(H-1)}$  span the

components, 
$$\Lambda$$
,  $\Xi$  and  $\Gamma$ , of  $\Omega_{H}(\boldsymbol{\theta}^{(H-1)})$ ; that is:  

$$\Lambda = \{ \alpha_{\tilde{\mathbf{w}}}(\boldsymbol{\theta}^{(H-1)}) | \tilde{\mathbf{w}} \in \mathbb{R}^{L+1} \},$$

$$\Xi = \{ \beta_{(v,w)}(\boldsymbol{\theta}^{(H-1)}) | (v,w) \in \mathbb{R}^{2} \}.$$
(19)  

$$\Gamma = \{ \gamma_{\lambda}(\boldsymbol{\theta}^{(H-1)}) | \lambda \in \mathbb{R} \}.$$

## 3. Critical points of the MLP model

## 3.1. Learning and critical points

Generally, the optimum parameter cannot be calculated analytically when the model is nonlinear. Some numerical optimization method is needed to obtain its approximation. One widely used method is the steepest descent method, which leads to a learning rule given by:

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \delta \frac{\partial E_H(\boldsymbol{\theta}(t))}{\partial \boldsymbol{\theta}}, \qquad (20)$$

where  $\delta$  is a learning rate. If  $\theta_*$  is the global minimum,  $(\partial E_H/\partial \theta)(\theta_*) = 0$  holds and the above learning rule stops there. However, we cannot always obtain the global minimum, since all the points that satisfy  $(\partial E_H/\partial \theta)(\theta) = 0$  are stationary points of Eq. (20). Such a point is called a *critical point* of  $E_H$ .

There are three types of critical point: a local minimum, a local maximum and a saddle point. A critical point  $\theta_0$  is called



(18)

Fig. 3. Embedding  $\beta_{(v,w)}$ .



Section with  $\widetilde{w}_1 = \widetilde{w}_2$ .

Fig. 4. Embedding  $\gamma_{\lambda}^+$ .

a *local minimum* (*maximum*) if there exists a neighborhood around  $\mathbf{\Theta}_0$  such that for any point  $\mathbf{\Theta}$  in the neighborhood  $E_H(\mathbf{\Theta}) \ge E_H(\mathbf{\Theta}_0) (E_H(\mathbf{\Theta}) \le E_H(\mathbf{\Theta}_0)$  holds, and called a *saddle* if it is neither a local minimum nor a local maximum, that is, if in an arbitrary neighborhood of  $\mathbf{\Theta}_0$  there is a point at which  $E_H$ is smaller than  $E_H(\mathbf{\Theta}_0)$  and a point at which  $E_H$  is larger than  $E_H(\mathbf{\Theta}_0)$ . It is well known that if the Hessian matrix at a critical point is strictly positive (negative) definite, the critical point is a local minimum (maximum), and if the Hessian has both positive and negative eigenvalues it is a saddle.

## 3.2. Existence of critical points

It is very natural to look for a critical point of  $E_H$  in the set  $\Omega_H = \pi_H^{-1}(\iota_{H-1}(\mathscr{S}_{H-1}))$ , because a critical point of  $E_{H-1}$  already satisfies some of the conditions of a critical point of  $E_H$ .

Let  $\mathbf{\theta}_{*}^{(H-1)} = (\zeta_{0*}, \zeta_{2*}, ..., \zeta_{H*}, \tilde{\mathbf{u}}_{2*}^{\mathrm{T}}, ..., \tilde{\mathbf{u}}_{H*}^{\mathrm{T}})^{\mathrm{T}} \in \Theta_{H-1}$  $-\Theta_{H-2}$  be a critical point of  $E_{H-1}$ . It really exists if we assume that the global minimum of  $E_{H-1}$  is isolated, which means it is not included in  $\Theta_{H-2}$ . This assumption is practically plausible, because, for a set of data which is fitted well with *H* hidden units, the optimum network with H - 1 hidden units has no redundant hidden units in general.

At the critical point, the following equations hold for  $2 \le j \le H$ ;

$$\frac{\partial E_{H-1}}{\partial \zeta_{0}} (\boldsymbol{\theta}_{*}^{(H-1)}) = \sum_{\nu=1}^{N} \frac{\partial \ell}{\partial z} (y^{(\nu)}, f^{(H-1)}(\mathbf{x}^{(\nu)}; \boldsymbol{\theta}_{*}^{(H-1)})) = 0,$$

$$\frac{\partial E_{H-1}}{\partial \zeta_{j}} (\boldsymbol{\theta}_{*}^{(H-1)})$$

$$= \sum_{\nu=1}^{N} \frac{\partial \ell}{\partial z} (y^{(\nu)}, f^{(H-1)}(\mathbf{x}^{(\nu)}; \boldsymbol{\theta}_{*}^{(H-1)})) \varphi(\tilde{\mathbf{u}}_{j_{*}}^{\mathrm{T}} \tilde{\mathbf{x}}^{(\nu)}) = 0,$$

$$\frac{\partial E_{H-1}}{\partial \tilde{\mathbf{u}}_{j}} (\boldsymbol{\theta}_{*}^{(H-1)})$$

$$= \zeta_{j*} \sum_{\nu=1}^{N} \frac{\partial \ell}{\partial z} (y^{(\nu)}, f^{(H-1)}(\mathbf{x}^{(\nu)}; \boldsymbol{\theta}_{*}^{(H-1)})) \varphi'(\tilde{\mathbf{u}}_{j_{*}}^{\mathrm{T}} \tilde{\mathbf{x}}^{(\nu)}) \tilde{\mathbf{x}}^{(\nu)\mathrm{T}} = \mathbf{0}^{\mathrm{T}},$$
(21)

We have two kinds of critical points.

**Theorem 1.** Let  $\gamma_{\lambda}$  be as in Eq. (18). Then, for any  $\lambda \in \mathbb{R}$ , the point  $\gamma_{\lambda}(\mathbf{\theta}_{*}^{(H-1)})$  is a critical point of  $E_{H}$ .

**Theorem 2.** Let  $\beta_{(v,w)}$  be as in Eq. (18). Then, for any  $w \in \mathbb{R}$ , the point  $\beta_{(0,w)}(\mathbf{\theta}^{(H-1)}_*)$  is a critical point of  $E_H$ .

These theorems are easily obtained if we consider the partial derivatives of  $E_H$ , which are given by

$$\frac{\partial E_H}{\partial v_0}(\boldsymbol{\theta}) = \sum_{\nu=1}^N \frac{\partial \ell}{\partial z} (y^{(\nu)}, f^{(H)}(\mathbf{x}^{(\nu)}; \boldsymbol{\theta})),$$

$$\frac{\partial E_H}{\partial v_j}(\boldsymbol{\theta}) = \sum_{\nu=1}^N \frac{\partial \ell}{\partial z} (y^{(\nu)}, f^{(H)}(\mathbf{x}^{(\nu)}; \boldsymbol{\theta})) \varphi(\tilde{\mathbf{w}}_j^{\mathrm{T}} \tilde{\mathbf{x}}^{(\nu)}), \quad (1 \le j \le H),$$

$$\frac{\partial E_H}{\partial \tilde{\mathbf{w}}_j}(\boldsymbol{\theta}) = v_j \sum_{\nu=1}^N \frac{\partial \ell}{\partial z} (y^{(\nu)}, f^{(H)}(\mathbf{x}^{(\nu)}; \boldsymbol{\theta})) \varphi'(\tilde{\mathbf{w}}_j^{\mathrm{T}} \tilde{\mathbf{x}}^{(\nu)}) \tilde{\mathbf{x}}^{(\nu)\mathrm{T}}, \quad (1 \le j \le H).$$
(22)

Note that  $f^{(H)}(\mathbf{x}; \mathbf{\theta}) = f^{(H-1)}(\mathbf{x}; \mathbf{\theta}_*^{(H-1)})$  for  $\mathbf{\theta} = \gamma_{\lambda}(\mathbf{\theta}_*^{(H-1)})$  or  $\mathbf{\theta} = \beta_{(0,w)}(\mathbf{\theta}_*^{(H-1)})$ . It is easy to check that the conditions Eq. (21) make all the above derivatives zero.

The critical points in Theorems 1 and 2 consist of a line in  $\Theta_H$  if we move  $\lambda \in \mathbb{R}$  and  $w \in \mathbb{R}$ , respectively. Note that  $\alpha_{\tilde{\mathbf{w}}} = \beta_{(0,w)}$  if  $\tilde{\mathbf{w}} = (w, \mathbf{0}^T)^T$ . Thus, these two embeddings give the same critical point set. If  $\mathbf{\theta}$  is a critical point of  $E_H$ , so is  $T_g(\mathbf{\theta})$  for any  $g \in G_H$ . We have many critical lines in  $\Theta_H$ .

The critical points in Theorems 1 and 2 do not cover all of the critical points of  $E_{H}$ . We consider the special subset of the critical points which appears because of the hierarchical structure of the model.

#### 4. Local minima of the MLP model

#### 4.1. A condition for the existence of local minima

In this section, we show a condition that a critical point in Theorem 1 is a local minimum or a saddle point. The usual sufficient condition of a local minimum using the Hessian matrix cannot be applied for a critical point in Theorem 1 and 2. The Hessian is singular, because a one-dimensional



Fig. 5. Critical set with local minima and plateaus.

set including the point shares the same value of  $E_H$  in common.

Let  $\mathbf{\theta}_{*}^{(H-1)}$  be a point in  $\Theta_{H-1}$ . We define the following  $(L+1) \times (L+1)$  symmetric matrix:

$$\mathscr{A}_{2} = \zeta_{2*} \sum_{\nu=1}^{N} \frac{\partial \boldsymbol{\ell}}{\partial z} (y^{(\nu)}, f^{(H-1)}(\mathbf{x}^{(\nu)}; \boldsymbol{\theta}_{*}^{(H-1)})) \varphi''(\tilde{\mathbf{u}}_{2*}^{\mathsf{T}} \tilde{\mathbf{x}}^{(\nu)}) \tilde{\mathbf{x}}^{(\nu)} \tilde{\mathbf{x}}^{(\nu)\mathsf{T}}.$$
(23)

**Theorem 3.** Let  $\boldsymbol{\theta}_{*}^{(H-1)}$  be a local minimum of  $E_{H-1}$  such that the Hessian matrix at  $\boldsymbol{\theta}_{*}^{(H-1)}$  is positive definite. Let  $\gamma_{\lambda}$  be defined by Eq. (18), and  $\Gamma = \{\boldsymbol{\theta}_{\lambda} \in \boldsymbol{\Theta}_{H} | \boldsymbol{\theta}_{\lambda} = \gamma_{\lambda}(\boldsymbol{\theta}_{*}^{(H-1)}), \lambda \in \mathbb{R}\}$ . A matrix  $A_{2}$  is defined by Eq. (23). If  $A_{2}$  is positive (negative) definite, any point in the set  $\Gamma_{0} = \{\boldsymbol{\theta}_{\lambda} \in \Gamma | \lambda(1 - \lambda) > 0(<0)\}$  is a local minimum of  $E_{H}$  and any point in  $\Gamma - \Gamma_{0}$  is a saddle. If  $A_{2}$  has both positive and negative eigenvalues, all the points in  $\Gamma$  are saddle points.

For the proof, see Appendix A.

Local minima given by Theorem 3, if any, appear as one or two segments in a line. It is interesting that such a local minimum can be changed into a saddle point without altering the function  $f_{\theta}^{(H)}$  when the point moves in the segment. Fig. 5 illustrates the error surface around this critical set. We show only two coordinate axes for variables: one is the direction along  $\Gamma$  and the other is the direction that attains the minimum and maximum values at the points on  $\Gamma$ . Each point that looks like a maximum in the figure is a saddle point in reality.

Note that, if  $\theta$  is a local minimum given by Theorem 3 the image of the point by any transform in  $G_H$  is also a local

minimum. This can be easily proved because the local property of  $G_H$  around the point does not change by the transform. Therefore, the error function has many line segments of local minima if the condition of Theorem 3 holds.

The critical points in Theorem 2 do not give local minima.

**Theorem 4.** Any critical point given by Theorem 2 is a saddle.

For the proof, see Appendix B.

The statements of Theorems 3 and 4 are also valid if we consider the transform of the embedded point by any  $g \in G_H$ . This can be proved easily because the local property around the point is not changed by any transform in  $G_H$ . There are many saddle line segments, and line segments of local minima if any.

## 4.2. Plateaus

We have proved that, when  $A_2$  is positive or negative definite, there exists a one-dimensional submanifold  $\Gamma$  of critical points. The output function is the same in  $\Gamma$ . The set  $\Gamma$  is divided into two parts  $\Gamma_0$  and  $\Gamma - \Gamma_0$ , where  $\Gamma_0$  consists of local minima and  $\Gamma - \Gamma_0$  saddles.

If we map to the function space,  $\pi_H(\Gamma)$  consists of a single point which is the common function  $f_{\theta^{(H)}}^{(H)} \in \mathscr{S}_H$ . Therefore, if we consider the cost function  $E_H$  as a function on  $\mathscr{S}_H$ ,  $\pi_H(\Gamma)$  is a saddle, because  $E_H$  takes both larger and smaller values than  $E_H(\theta^{(H)})$  in any neighborhood of  $f_{\theta^{(H)}}^{(H)}$  in  $\mathscr{S}_H$ .

It is interesting to see that  $\Gamma_0$  is attractive in its neighborhood. Hence, any point in its small neighborhood is attracted to  $\Gamma_0$ . However, if we use online learning, in



Fig. 6. A local minimum in MLP (L = 1, H = 2).

which the parameter is updated with a training datum presented one by one, the point attracted to  $\Gamma_0$  fluctuates randomly along  $\Gamma_0$  by the learning dynamics. It eventually escapes from  $\Gamma$  when it reaches  $\Gamma - \Gamma_0$ . This takes a long time because of the nature of random fluctuation. This explains that this type of critical points are serious plateaus. This is a new type of saddle which has so far not remarked in nonlinear dynamics. This type of "intrinsic saddle" is given rise to by the singular structure of the topology of  $\mathcal{S}_H$ .

## 4.3. Remarks

The only property of tanh used in this paper is that it is odd. Kůrkova and Kainen ((1994); Theorem 8) introduced the notion of affinely recursive functions, and proved that if the activation function is odd or even and is not affinely recursive, the functionally equivalent parameters are given by interchanges and sign flips, neglecting compensation of constant. A function  $\varphi : \mathbb{R} \to \mathbb{R}$  is not affinely recursive if and only if it has a nontrivial affine relation  $\varphi(t) = a\varphi(wt + u) + b$ for  $a, w \neq 0$  and an affine relation  $\sum_{i=1}^{m} a_i \varphi(w_i t + u_i) + b = 0$ of more than three components can be decomposed into affine relations of two components (For the precise definition, see Kůrkova and Kainen (1994).) Using this result, we can deduce that  $\Omega_H$  is the same as for MLP models with an odd or even activation function that is not affinely recursive, and can determine the transform group for such MLP models. The group is still the same as  $G_H$ , while we must replace the definition of a sign flip by  $(v_i, \mathbf{w}_i) \mapsto (v_i, -\mathbf{w}_i)$ for an even-activation function. Similar arguments in Section 2.2 are valid, and Theorems 1-4 also hold with necessary modifications of the statements. A typical activation function like the logistic function and Gaussian function can be converted by an affine transform to an odd or even function that is not affinely recursive. Therefore, the results obtained in the above are applicable to a wide class of three-layer models.

### 4.4. Numerical simulations

We have tried numerical simulations to exemplify local minima given by Theorem 3 and plateaus described in Section 4.2.

In the first simulation, we use a network with one input unit, one output unit and two hidden units. We do not use bias terms for simplicity. Note that there always exist local minima in this case, since  $A_2$  is a scalar. We use the logistic function  $\varphi(t) = 1/(1 + e^{-t})$  as the activation function, and the mean square error  $l(y, z) = 1/2||y - z||^2$  for the loss function. To obtain training data, 100 input data are generated using a normal distribution with 0 as its mean and 4.0 as its variance, and corresponding output data are obtained as y =f(x) + Z, where  $f(x) = 2\varphi(x) - \varphi(4x)$  and Z is a random variable subject to the normal variable with 0 as its mean and  $10^{-4}$  as its variance. For a fixed set of training data, we numerically calculate the global minimum of MLP with one hidden unit using the steepest descent method. We update the parameter 20 000 times, and use the final state as the global minimum. Even if we try several different initial conditions the obtained results are almost the same. Therefore, we can consider it as an approximation of the global minimum  $\mathbf{\theta}_{*}^{(1)}$  with high accuracy. The parameter is given by  $\zeta_{2*} = 0.984$  and  $u_{2*} = 0.475$ . In this case, we have  $A_2 = 1.910 > 0$ . Then, any point in the set  $\Gamma_0 =$ { $(v_1, v_2, w_1, w_2)|v_1 + v_2 = \zeta_{2*}, v_1v_2 > 0, w_1 = w_2 = u_{2*}$ } is a local minimum. We set  $v_1 = v_2 = \zeta_{2*}/2$  as  $\theta_{\lambda}(\lambda = 1/2)$ , and evaluate the values of  $E_2$  at a million points around  $\theta_{\lambda}$ , which are generated using a four-dimensional normal distribution with  $\theta_{\lambda}$  as its mean and  $10^{-6}I_4$  as its variance–covariance matrix. As a result, all these values are larger than  $E(\mathbf{\theta}_{\lambda})$ . This experimentally verifies that  $\mathbf{\theta}_{\lambda}$  is a local minimum. The graphs of the target function f(x) and the function given by the local minimum  $f(x; \theta_*^{(1)})$  are shown in Fig. 6.

In the second simulation, we use a network with two input units, one output unit and three hidden units. We do not use bias terms also in this simulation. The  $2 \times 2$  matrix  $A_2$  can have both of a negative and a positive eigenvalue at the same time. The activation function is tanh, and the set of input data is 100 independent samples from the normal distribution with 0 as its mean and  $25 \times I_2$  as its covariance matrix. The target function is given by a function in the model, which is defined by  $v_1 = v_2 = v_3 = 1$ ,  $\mathbf{w}_1 = (2, 1)^T$ ,  $\mathbf{w}_2 = (1, -1)^T$  and  $\mathbf{w}_3 = (1, -1)^T$  $(0.5, 0)^{\mathrm{T}}$ . We numerically obtain the global minimum of the model with two hidden units,  $\theta_*^{(2)}$ , in the similar method to the first simulation. There are many cases in which the matrix  $A_2$ has a negative and a positive eigenvalue, but for some sets of training data and initial parameters we can find the matrix positive or negative definite. Fig. 7 shows the graph of a function given by one of such local minima and the graph of the target function. The parameter of this local minimum is  $\zeta_{1*} = 1.864, \ \zeta_{2*} = -1.158, \ \mathbf{u}_{1*} = (-0.680, 0.247)^{T}$  and  $\mathbf{u}_{2*} = (-0.905, -1.158)^{T}$ . We numerically confirmed, in the same way as in the first simulation, that this is really a local minimum.



Fig. 7. A local minimum and the target in MLP (L = 2, H = 3).

Next, we have tried to verify that this local minimum causes a plateau. In this simulation, we use online learning, in which the parameter is updated with respect to only one training data that is selected at that time. All of the training data are used by turns, and training is repeated cyclically. We observe the behavior of the parameter after setting it close to the one that gives the local minimum. Fig. 8 is the graph of the value of error function  $E_3(\mathbf{\theta})$  during learning, which shows a typical plateau until about 50 000 iterations. One sequence of presenting all data is counted as one iteration in this figure. We can see a very long time interval, in which the error function decreases very slowly, and a

sudden steep decrease of the training error. Fig. 9 shows the behavior of the parameter  $\mathbf{w}_1$  and  $\mathbf{w}_2$ . They move close to the parameter  $\mathbf{u}_{1*}$ , which gives the local minimum, and suddenly go away from it. This simulation verifies that local minima given by Theorem 3 can give rise to plateaus as we discussed in Section 4.2.

# 5. Conclusion

We investigated the geometric structure of the parameter space of multilayer perceptrons with H - 1 hidden units



Fig. 8. Value of the error function during learning.

embedded in the parameter space of H hidden units. Based on the structure, we found a finite family of critical point sets of the error surface. We showed that a critical point of a smaller network can be embedded into the parameter space as a critical point set of a one-dimensional affine space in two ways. We further elucidated a condition that a point in the image of one embedding is a local minimum, and showed that the image of the other embedding is a saddle. From this result, we see that under one condition there exist local minima as line segments in the parameter space, which cause serious plateaus because all points around the set of local minima once converge to it and have to escape from it by random fluctuation. These results are not dependent on the specific form of activation functions nor the loss functions.

We consider only networks with one output unit. The extension of the result on existence of local minima is not straightforward. The image of the embedding  $\gamma_{\lambda}$  form a critical line even in the *M*-dimensional output case. However, the critical line is contained in the *M*-dimensional affine space defined by  $\mathbf{v}_1 + \mathbf{v}_2 = \boldsymbol{\zeta}_{2*}$ , in which a point does not give a critical point in general, but defines the same input–output function as the critical line. From Lemma 1



Fig. 9. Behavior of parameters.

in Appendix A, we see that any point in the critical line is a saddle. We have not yet known about existence of local minima in the case of multiple output units.

Theorems 3 and 4 mean that the critical points are saddles in many cases. It is very important to know a condition on the positive or negative definiteness of  $A_2$ . This is a difficult problem, because it deeply depends on the relation between the global minimum in  $\Theta_{H-1}$ , and on the target and randomness of training data. From the practical point of view, it is meaningful to see whether the saddle points in Theorems 3 and 4 are the only reason of plateaus. If this is true, we can effectively avoid them by the method of natural gradient (Amari, 1998; Amari, Park & Fukumizu, 2000; Rattray, Saad & Amari, 1998; Yang & Amari, 1998), because it enlarges the gradient of the repulsive direction from by multiplying the inverse of the almost singular Fisher information matrix. However, all of the above problems are left open.

### Appendix A. Proof of Theorem 3

**Proof.** For simplicity, we change the order of the components of  $\boldsymbol{\theta}^{(H)}$  and  $\boldsymbol{\theta}^{(H-1)}$  as  $(v_1, v_2, \tilde{\mathbf{w}}_1^{\mathrm{T}}, \tilde{\mathbf{w}}_2^{\mathrm{T}}, v_0, v_3, ..., v_H, \tilde{\mathbf{w}}_3^{\mathrm{T}}, ..., \tilde{\mathbf{w}}_H^{\mathrm{T}})^{\mathrm{T}}$  and  $(\zeta_2, \tilde{\mathbf{u}}_2^{\mathrm{T}}, \zeta_0, \zeta_3, ..., \zeta_H, \tilde{\mathbf{u}}_3^{\mathrm{T}}, ..., \tilde{\mathbf{u}}_H^{\mathrm{T}})^{\mathrm{T}}$ , respectively. We introduce a new coordinate system of  $\Theta_H$  to see the embedding  $\gamma_{\lambda}$  more explicitly. Let  $(\xi_1, \mathbf{\eta}^T, \xi_2, \mathbf{b}^T, v_0, v_3, ..., v_H, \tilde{\mathbf{w}}_3^T, ..., \tilde{\mathbf{w}}_H^T)^T$  be a coordinate system of  $\Theta_H - \{\mathbf{\theta}^{(H)} | v_1 + v_2 = 0\}$ , where:

$$\xi_{1} = v_{1} - v_{2}, \qquad \mathbf{\eta} = \frac{1}{v_{1} + v_{2}} (\tilde{\mathbf{w}}_{1} - \tilde{\mathbf{w}}_{2}),$$

$$\xi_{2} = v_{1} - v_{2}, \qquad \mathbf{b} = \frac{v_{1}}{v_{1} + v_{2}} \tilde{\mathbf{w}}_{1} + \frac{v_{2}}{v_{1} + v_{2}} \tilde{\mathbf{w}}_{2}.$$
(A1)

This is well defined as a coordinate system since the inverse is given by:

Using this coordinate system, the embedding  $\gamma_{\lambda}$  is expressed as:

$$\gamma_{\lambda} : (\zeta_2, \tilde{\mathbf{u}}_2^{\mathrm{T}}, \zeta_0, \zeta_3, ..., \zeta_H, \tilde{\mathbf{u}}_3^{\mathrm{T}}, ..., \tilde{\mathbf{u}}_H^{\mathrm{T}})^{\mathrm{T}}$$

$$\mapsto ((2\lambda - 1)\zeta_2, \mathbf{0}^{\mathrm{T}}, \zeta_2, \tilde{\mathbf{u}}_2^{\mathrm{T}}, \zeta_2, \zeta_3, ..., \zeta_H, \tilde{\mathbf{u}}_3^{\mathrm{T}}, ..., \tilde{\mathbf{u}}_H^{\mathrm{T}})^{\mathrm{T}}.$$
(A3)

Note that in this definition we use the order of the components introduced at the beginning of the proof.

Let  $(\zeta_{2*}, \tilde{\mathbf{u}}_{2*}^{\mathrm{T}}, \zeta_{0*}, \zeta_{3*}, ..., \zeta_{H*}, \tilde{\mathbf{u}}_{3*}^{\mathrm{T}}, ..., \tilde{\mathbf{u}}_{H*}^{\mathrm{T}})^{\mathrm{T}}$  be the component of  $\boldsymbol{\theta}_{*}^{(H-1)}$ . The critical point set  $\Gamma$  is a one-dimensional affine space parallel to  $\xi_1$ -axis with  $\eta = 0$ ,  $\xi_2 = \zeta_{2*}$ ,  $\mathbf{b} = \tilde{\mathbf{u}}_{2*}, \ v_0 = \zeta_{0*}, \ v_j = \zeta_{j*} (3 \le j \le H) \ \text{and} \ \tilde{\mathbf{w}}_j = \tilde{\mathbf{u}}_{j*} (3 \le J \le H)$  $j \leq H$ ).

Let  $\xi_{1*}$  be the  $\xi_1$  component of  $\theta_{\lambda}$ , and  $V_{\xi_{1*}}$  be a comple-

ment of  $\Gamma$  defined by:

$$V_{\xi_{1_*}} := \{ (\xi_1, \mathbf{\eta}^{\mathrm{T}}, \xi_2, \mathbf{b}^{\mathrm{T}}, v_0, v_3, \dots, v_H, \tilde{\mathbf{w}}_3^{\mathrm{T}}, \dots, \tilde{\mathbf{w}}_H^{\mathrm{T}})^{\mathrm{T}} \in \Theta_H | \xi_1 = \xi_{1*} \}.$$
(A4)

We have  $\Gamma \cap V_{\xi_{1_*}} = \mathbf{0}_{\lambda}$ . If  $\mathbf{0}_{\lambda}$  is a local minimum in  $V_{\xi_{1_*}}$  for an arbitrary  $\mathbf{\theta}_{\lambda} \in \Gamma_0$ . it is a local minimum also in  $\Theta_H$ , since  $E_H$  has the same value on each point of. It is trivial that if  $\boldsymbol{\theta}_{\lambda}$ is a saddle point in  $V_{\xi_1}$ , it is a saddle also in  $\Theta_H$ . Thus, we can reduce the problem to the Hessian of  $E_H$  restricted on  $V_{\xi_{1*}}$ . We write it by  $\mathscr{G}_{\xi_{1*}}$ . From the definition of  $\eta$  and  $\xi_1$ , we have

Lemma 1. For any 
$$\boldsymbol{\theta} \in \{\boldsymbol{\theta}^{(H)} \in \boldsymbol{\Theta}_{H} | \boldsymbol{\eta} = \boldsymbol{0}\},\$$
  
$$\frac{\partial f}{\partial \boldsymbol{\eta}}(\mathbf{x}; \boldsymbol{\theta}) = \boldsymbol{0} \text{ and } \frac{\partial f}{\partial \xi_{1}}(\mathbf{x}; \boldsymbol{\theta}) = 0$$
(A5)

hold.

From Eq. (A3), we have also  $(\partial f/\partial \mathbf{b})(\mathbf{\theta}_{\lambda}) = \mathbf{0}$  and  $(\partial f/\partial \xi_2)(\mathbf{\theta}_{\lambda}) = 0$  (this is another proof of Theorem 2). Therefore, the second derivative of  $E_H$  at  $\mathbf{\theta}_{\lambda}$  can be written as:

$$\nabla \nabla E_{H}(\boldsymbol{\theta}_{\lambda}) \sum_{\nu=1}^{N} \frac{\partial \boldsymbol{\ell}}{\partial \boldsymbol{z}} (\mathbf{y}^{(\nu)}, f(\mathbf{x}^{(\nu)}, \boldsymbol{\theta}_{\lambda})) \nabla \nabla f(\mathbf{x}^{(\nu)}, \boldsymbol{\theta}_{\lambda}).$$
(A6)

Let  $\omega$  represent one of the coordinate components in  $(\boldsymbol{\xi}_1, \boldsymbol{\eta}^{\mathrm{T}}, \boldsymbol{\xi}_2, \mathbf{b}^{\mathrm{T}}, v_0, v_3, \dots, v_H, \tilde{\mathbf{w}}_3^{\mathrm{T}}, \dots, \tilde{\mathbf{w}}_H^{\mathrm{T}})$ . From Lemma 1, at any point  $\theta \in \{\eta = 0\}$ , the second derivative  $(\partial^2 f/\partial \xi_1 \partial \omega)(\mathbf{\theta}) = \mathbf{0}$  and  $(\partial^2 f/\partial \mathbf{\eta} \partial \omega)(\mathbf{\theta}) = \mathbf{0}$  unless  $\omega =$  $\eta_i$  (1  $\leq j \leq L + 1$ ). Combining this fact with the expression of Eq. (A3), we have:

$$\mathscr{G}_{\xi_{1*}} = \begin{pmatrix} \frac{\partial^2 E_H}{\partial \boldsymbol{\eta} \ \partial \boldsymbol{\eta}} (\boldsymbol{\theta}_{\lambda}) & 0\\ 0 & \frac{\partial^2 E_{H-1}}{\partial \boldsymbol{\theta}^{(H-1)} \ \partial \boldsymbol{\theta}^{(H-1)}} (\boldsymbol{\theta}_*^{(H-1)}) \end{pmatrix}. \quad (A7)$$

By simple calculation we can derive the following:

**Lemma 2.** For any  $\boldsymbol{\theta} \in \{\boldsymbol{\theta}^{(H)} \in \boldsymbol{\Theta}_H | \boldsymbol{\eta} = \boldsymbol{0}\},\$ 

$$\frac{\partial^2 f}{\partial \boldsymbol{\eta} \, \partial \boldsymbol{\eta}}(\mathbf{x}, \boldsymbol{\theta}) = v_1 v_2 \frac{\partial^2 f}{\partial \mathbf{b} \, \partial \mathbf{b}}(\mathbf{x}, \boldsymbol{\theta}) = v_1 v_2 \xi_2 \varphi''(\mathbf{b}^{\mathrm{T}} \tilde{\mathbf{x}}) \tilde{\mathbf{x}} \tilde{\mathbf{x}}^{\mathrm{T}}$$
(A8)

holds.

From this lemma, we have  $(\partial^2 E_H / \partial \eta \, \partial \eta)(\theta_{\lambda}) =$  $\lambda(1-\lambda)\zeta_{2*}^2 A_2$ . From the assumption, all the eigenvalues of  $(\partial^2 E_{H-1}/\partial \mathbf{\theta}^{(H-1)} \partial \mathbf{\theta}^{(H-1)})(\mathbf{\theta}_*^{(H-1)})$  are positive and  $\zeta_{2*} \neq$ 0. Thus, if  $A_2$  is positive or negative definite, all the eigenvalues of  $\mathscr{G}_{\xi_{1*}}$  at a point in  $\Gamma_0$  are positive, which means  $\boldsymbol{\theta}_{\lambda}$ is a local minimum in  $\Theta_{H}$ . If  $A_2$  has positive and negative eigenvalues, so does  $\mathscr{G}_{\xi_{1*}}$  except for two points given by  $\lambda = 0, 1$ . Then, all the points in  $\Gamma - \overline{\Gamma}_0$  are saddle points. As for the two boundary points of  $\Gamma_0$ , any neighborhood of them contains a point of  $\Gamma - \overline{\Gamma}_0$ . Thus, the neighborhood includes a point attaining larger  $E_H$  than  $E_H(\mathbf{\theta}_{\lambda})$  and a point attaining smaller  $E_H$  than  $E_H(\mathbf{\theta}_{\lambda})$ . Thus, they are also saddle points, and this completes the proof.  $\Box$ 

### Appendix B. Proof of Theorem 4

**Proof.** First, we show the following lemma.

**Lemma 3.** Let  $E(\mathbf{\theta})$  be a function of class  $C^l$ , and  $\mathbf{\theta}_*$  be a critical point of  $E(\mathbf{\theta})$ . If in any neighborhood of  $\mathbf{\theta}_*$  there exists a point  $\mathbf{\theta}$  such that  $E(\mathbf{\theta}) = E(\mathbf{\theta}_*)$  and  $(\partial E/\partial \mathbf{\theta})(\mathbf{\theta}) \neq \mathbf{0}$ , then  $\mathbf{\theta}_*$  is a saddle point.

**Proof.** Let *U* be a neighborhood of  $\mathbf{\theta}_*$ . From the assumption, we have a point  $\mathbf{\theta}_1 \in U$  such that  $E(\mathbf{\theta}_1) < E(\mathbf{\theta}_*)$  and a point  $\mathbf{\theta}_2 \in U$  such that  $E(\mathbf{\theta}_2) > E(\mathbf{\theta}_*)$ . This means  $\mathbf{\theta}_*$  is a saddle point.  $\Box$ 

Back to the proof of Theorem 4, note that  $\beta_{(0,w)}(\mathbf{\theta}_*^{(H-1)}) \in \{\alpha_{\tilde{\mathbf{w}}}(\mathbf{\theta}_*^{(H-1)}) | \tilde{\mathbf{w}} \in \mathbb{R}^{L+1}\}$ . In other words, the critical line in Theorem 2 is embedded in an L + 1 dimensional plane that gives the same function as the critical line. However, the point  $\alpha_{\tilde{\mathbf{w}}}(\mathbf{\theta}_*^{(H-1)})$  is not a critical point for  $\mathbf{w} \neq \mathbf{0}$ , because  $\partial E_H / \partial v_1 \neq 0$  in general. Thus,  $\beta_{(0,w)}(\mathbf{\theta}_*^{(H-1)})$  satisfies the assumption of Lemma 3.  $\Box$ 

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