A Note on Connectivity of Sublevel Sets in Deep Learning

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Abstract

It is shown that for deep neural networks, a single wide layer of width $N + 1$ ($N$ being the number of training samples) suffices to prove the connectivity of sublevel sets of the training loss function. In the two-layer setting, the same property may not hold even if one has just one neuron less (i.e. width $N$ can lead to disconnected sublevel sets).

1 Introduction

Geometry of neural network loss landscape has been studied via the analysis of the global optimality of local minima [1, 2, 5, 8, 9, 14], the existence of a continuous descending path to a global optimum [3, 7, 10, 11, 13], the connectivity of dropout-stable solutions [6, 12], and the topology of sublevel sets [7, 13]. In this paper, we improve the result of [7].

In particular, [7] shows that for a general class of convex loss functions (e.g. cross-entropy loss, square loss), and for any training data with distinct samples, all the sublevel sets of the (empirical) training loss are connected if the (deep) network satisfies the following conditions:

1. The first hidden layer has $2N$ neurons ($N$ being the number of training samples), and the other layers have non-increasing widths towards the output layer (a.k.a. pyramidal network).

2. The activation is piecewise linear (excluding the linear ones), and strictly monotonic.

On the one hand, we know that the connectivity of sublevel sets implies the following: (i) the loss surface has no bad local valleys, and that (ii) all the global minima are connected within a unique global valley. On the other hand, we also know that for the property (i) to hold, a single layer of width $N$ suffices [10, 13]. This raises an intriguing question of how the loss function evolves when the number of neurons varies between $N$ and $2N$ neurons. This paper aims to bridge this gap.

Main Contribution. We improve the width condition of the previous result from $2N$ to $N + 1$ for deep architectures. That is, if the width of the first layer is at least $N + 1$, and the other assumptions hold as above, then every sublevel set of the empirical loss is connected. Furthermore, in the two-layer setting, we show that the same statement is wrong if one has one neuron less (i.e. with just $N$ neurons, the loss can have disconnected sublevel sets). This shows that our width condition $N + 1$ is tightest possible for this case unless additional assumptions on the data/network are made.

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Preliminaries. Consider an $L$-layer neural network where the widths of the layers are given by $(n_0, \ldots, n_L)$. Here, $n_0$ and $n_L$ are input and output dimension respectively, and the rest are the hidden layers. Let $N$ be the number of training samples. Let $X \in \mathbb{R}^{N \times n_0}$ and $Y \in \mathbb{R}^{N \times n_L}$ be the training data. The feature matrices $F_l \in \mathbb{R}^{N \times n_l}$ are given by

$$F_l = \begin{cases} X & l = 0, \\ \sigma(F_{l-1}W_l + 1_N b_l^T) & l \in [L - 1], \\ F_{l-1}W_l & l = L, \end{cases}$$

where $W_l \in \mathbb{R}^{n_{l-1} \times n_l}, b_l \in \mathbb{R}^{n_l}$, and $\sigma: \mathbb{R} \rightarrow \mathbb{R}$ is the activation function which is applied componentwise. Let $\theta = (W_l, b_l)_{l=1}^L$ be the set of parameters. The training loss is defined as

$$\Phi(\theta) = \Psi(F_L(\theta), Y)$$

where the function $\Psi(\hat{Y}, Y)$ is assumed to be convex w.r.t. the first argument.

Assumption 1.1 $\sigma$ is strictly monotonic and $\sigma(\mathbb{R}) = \mathbb{R}$.

Assumption 1.2 There do not exist non-zero coefficients $(\lambda_i, a_i)_{i=1}^p$ with $a_i \neq a_j \forall i \neq j$ such that $\sigma(x) = \sum_{i=1}^p \lambda_i \sigma(x - a_i)$ for every $x \in \mathbb{R}$.

Assumption 1.2 is satisfied for every piecewise linear activation function of interest (e.g. ReLU and Leaky-ReLU), see [7]. In the following, the $\alpha$-sublevel set of the training function is defined as

$$\forall \alpha \in \mathbb{R} : L_\alpha = \{ \theta \mid \Phi(\theta) \leq \alpha \}.$$  

The $\alpha$-level set is defined as $\{ \theta \mid \Phi(\theta) = \alpha \}$. A subset $A \subseteq \mathbb{R}^n$ is called connected if for any $x, y \in A$, there exists a continuous curve (path) $c: [0, 1] \rightarrow A$ such that it holds $c(0) = x$ and $c(1) = y$.

2 Some Helpful Results

Theorem 2.1 [7] Let Assumption 1.1 hold, rank$(X) = N$ and $n_1 > \ldots > n_L$ where $L \geq 2$. Then,

1. Every sublevel set of $\Phi$ is connected. And $\Phi$ can attain any value arbitrarily close to inf$_\theta \Phi(\theta)$.

2. Every non-empty connected component of every level set of $\Phi$ is unbounded.

Lemma 2.2 [7] Let $(X, W, b, V) \in \mathbb{R}^{N \times d} \times \mathbb{R}^{d \times n} \times \mathbb{R}^n \times \mathbb{R}^{n \times p}$. Let Assumption 1.2 hold. Suppose that $n \geq N$ and $X$ has distinct rows. Let $Z = \sigma(XW + 1_N b^T)V$. There is a continuous curve $c: [0, 1] \rightarrow \mathbb{R}^{d \times n} \times \mathbb{R}^n \times \mathbb{R}^{n \times p}$ with $c(\lambda) = (W(\lambda), b(\lambda), V(\lambda))$ satisfying:

1. $c(0) = (W, b, V)$.

2. $\sigma\left(\sum_{i=1}^p \lambda_i b(\lambda)^T\right) V(\lambda) = Z, \forall \lambda \in [0, 1]$.

3. rank $\left(\sigma\left(\sum_{i=1}^p \lambda_i b(\lambda)^T\right)\right) = N$.  

Lemma 2.3 Let $F \in \mathbb{R}^{N \times n}, W \in \mathbb{R}^{n \times p}$. Let $I$ be a subset of columns of $F$, and $\bar{I}$ its complement such that every column in $\bar{I}$ belongs to the linear span of all the columns in $I$. Then there exists a continuous curve $c: [0, 1] \to \mathbb{R}^{n \times p}$ which satisfies the following:

1. $c(0) = W$ and $Fc(\lambda) = FW, \forall \lambda \in [0, 1]$.
2. Let $W' = c(1)$. Then $W'(\bar{I}, :) = 0$.

Proof: Let $r = \text{rank}(F) < n$. There exists $E \in \mathbb{R}^{r \times (n-r)}$ so that $F(:, \bar{I}) = F(:, I) E$. Let $P \in \mathbb{R}^{n \times n}$ be a permutation matrix which permutes the columns of $F$ according to $I$ so that we can write $F = [F(:, I), F(:, \bar{I})] P$. Consider the continuous curve $c: [0, 1] \to \mathbb{R}^{n \times p}$ defined as

$$c(\lambda) = P^T \left[ W(I, :) + \lambda E W(\bar{I}, :) \right] (1 - \lambda) W(\bar{I}, :)$$

It holds $c(0) = P^T \left[ W(I, :) \right] = W$. For every $\lambda \in [0, 1]$:

$$Fc(\lambda) = [F(:, I), F(:, \bar{I})] PP^T \left[ W(I, :) + \lambda E W(\bar{I}, :) \right] (1 - \lambda) W(\bar{I}, :)$$

$$= F(:, I)W(I, :) + F(:, \bar{I})W(\bar{I}, :) = FW.$$

The second statement follows by noting that $c(\lambda)(\bar{I}, :) = (1 - \lambda)W(\bar{I}, :)$.

Lemma 2.4 Let $F \in \mathbb{R}^{N \times n}, W \in \mathbb{R}^{n \times p}$. Let $k, j \in [n]$ be a pair of distinct columns of $W$ such that $W_j = 0$ and $F_j = F_k$. Then there exists a continuous curve $c: [0, 1] \to \mathbb{R}^{n \times p}$ which satisfies that:

1. $c(0) = W$ and $Fc(\lambda) = FW, \forall \lambda \in [0, 1]$.
2. Let $U = c(1)$. Then $c(1)(k,:) = U_k = 0$.

Proof: Take the path $c$ to be

$$c(\lambda)(p,:) = \begin{cases} W_p: & p \neq j, k \\ (1 - \lambda)W_k: & p = k \\ \lambda W_k: & p = j \end{cases}$$

Then, it is easy to check that $c$ satisfies the lemma.

3 Sufficiency of Width $N + 1$ for Deep Networks

Our main result is the following.

Theorem 3.1 Consider an $L$-layer network. Let Assumption 1.1 and Assumption 1.2 hold. Suppose that $n_1 \geq N + 1$ and $n_2 > \ldots > n_L$. Then every sublevel set of $\Phi$ is connected, and every non-empty connected component of every level set of $\Phi$ is unbounded.
We want to show that there is a connected path between $\theta$ and $\theta'$ on which the loss is not larger than $\alpha$. The output at the first layer is given by

$$F_1 := F_1(\theta) = \sigma([X, 1_N][W^T_1, b_1]^T),$$

$$F'_1 := F_1(\theta') = \sigma([X, 1_N][W'^T_1, b'_1]^T).$$

First, by applying Lemma 2.2 to $(X, W_1, b_1, W_2)$, we can assume that $F_1$ has full rank. Otherwise, there is a path of constant loss from $\theta$ to some other point where this property is satisfied. Similarly, one can also assume that rank($F'_1$) = $N$. In the remaining, we assume w.l.o.g. that the first $N$ columns of $F_1$ are linearly independent. Let $\tilde{W}_1 = [W^T_1, b_1]^T$.

As the second step, we fix $\theta'$ and move $\theta$ along another path of constant loss such that at the end of this path, $\theta$ and $\theta'$ have the same parameter values at the first layer. To do so, we use induction. Assume that we have already made the first $k - 1$ columns of $\tilde{W}_1$ coincide with $\tilde{W}'_1$. Let us show how to do this for the $k$-th column. Let $j'$ be the smallest index such that $j' \geq k$ and $(F_1)_{j',j'} \in \text{Span}\{(F_1)_{j,p}\}_{p=1}^{j-1}$. Such an index always exists because of the following reason: for $k - 1 \geq N$, this simply follows from the fact that the first $N$ columns of $F_1$ are linearly independent by induction assumption; and for $k - 1 < N$, it follows from the fact that there are at most $N$ independent columns but we have more columns to choose than $N$ (i.e. $n_1 > N$). Now, by the choice of $j'$, we have that $(F_1)_{j',j'}$ belongs to the linear span of the first $j' - 1$ columns. Thus by using Lemma 2.3, we can find a path on $W_2$ such that the output stays invariant and we obtain at the end of the path $(W_2)_{j',j'} = 0$. Now, since the output weights of neuron $j'$ is zero, we can continuously change its incoming weights to any target value we want without affecting the output/loss. Consider to do this so that we obtain $(\tilde{W}_1)_{j',j'} = (\tilde{W}_1)_{j,k}$. This gives us $(F_1)_{j,k} = (F_1)_{j',j'}$. Now, the neurons $\{k, j'\}$ satisfy the conditions of Lemma 2.4 thus we can follow a path of constant loss to obtain $(W_2)_{j,k} = 0$. Finally, take the direct line segment between $(\tilde{W}_1)_{j,k}$ and $(\tilde{W}'_1)_{j,k}$ to obtain $(\tilde{W}_1)_{j,k} = (\tilde{W}'_1)_{j,k}$.

The completion of the second step leaves us with $(W_1, b_1) = (W'_1, b'_1)$. Note that $\theta'$ is unchanged in the second step, so we still have from the earlier construction that rank($F_1(\theta')$) = $N$. Let $F_1 := F_1(\theta) = F_1(\theta')$. Then, by fixing $(W_1, b_1)$, one can view $F_1$ as the new training data for the subnetwork from layer 1 till layer $L$. This subnetwork and the new data $F_1$ satisfy all the conditions of Theorem 2.1 and so it follows that the loss function restricted to this subnetwork has connected sublevel sets. That means that there is a connected path between $(W_1, b_1)_{i=2}^{L-2}$ and $(W'_1, b'_1)_{i=2}^{L-2}$ on which the loss is not larger than $\alpha$. This further implies that a continuous path between $\theta$ and $\theta'$ exists in $L_\alpha$, and so $L_\alpha$ must be connected. 

\section{Necessity of Width $N + 1$ for Two-layer Networks}

The next result shows that a two-layer model with width $N$ may not have connected sublevel sets.

\textbf{Theorem 4.1} Consider a two-layer network where the width of the hidden layer satisfies $n_1 \leq N$. Let Assumption 1.2 hold. Let $(X, Y)$ be some training data such that the following conditions are satisfied: (i) there exists $n_1$ samples indexed by the subset $\mathcal{I} \subseteq [n_1]$ with $|\mathcal{I}| = n_1$, such that \{Y_{i}\}_{i \in \mathcal{I}} are linearly independent, (ii) the network can fit perfectly the training data, i.e. \(\exists \theta = (W_1, b_1, W_2) \text{ s.t. } \sigma(XW_1 + 1_N b_1^T)W_2 = Y\). Then, the set of global minima of $\Phi$ is disconnected.
Proof: Let $\theta$ be a global minimum. Recall that $F_1(\theta) = \sigma(XW_1 + 1_N\theta_1^T)$. Let us omit the argument and write just $F_1$. As $\theta$ is optimal, we have $(F_1)_{\mathcal{I}_2}W_2 = Y_{\mathcal{I}_2}$. By assumption, all the $n_1$ rows of $Y_{\mathcal{I}_2}$ are linearly independent, so the matrix $(F_1)_{\mathcal{I}_2}$ must have full rank $n_1$. As a remark, the existence of points in parameter space where $(F_1)_{\mathcal{I}_2}$ has full rank can be guaranteed by Lemma 2.2. Let $\theta'$ be obtained from $\theta$ by exchanging two neurons. Then, clearly $\theta'$ is also a global minimizer. Let $F'_1 = F_1(\theta')$. Then, $(F'_1)_{\mathcal{I}_2}$ can be obtained from $(F_1)_{\mathcal{I}_2}$ by exchanging two columns, so their determinants have opposite signs. Now, suppose by contradiction that $\theta$ and $\theta'$ are connected by a path of global minima $\theta(\lambda), \lambda \in [0, 1]$. By the above argument, it holds $\text{rank}((F_1(\theta(\lambda)))_{\mathcal{I}_2}) = n_1$. This implies that there is a continuous path from $(F_1)_{\mathcal{I}_2}$ to $(F'_1)_{\mathcal{I}_2}$ along which the matrix has full rank. This contradicts the fact that the set of full-rank matrices in $\mathbb{R}^{n_1 \times n_1}$ has two connected components, one with positive determinant and the other with negative determinant [3]. □

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