When Can Neural Networks Learn Connected Decision Regions?

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Abstract

Previous work has questioned the conditions under which the decision regions of a neural network are connected and further showed the implications of the corresponding theory to the problem of adversarial manipulation of classifiers. It has been proven that for a class of activation functions including leaky ReLU, neural networks having a pyramidal structure, that is no layer has more hidden units than the input dimension, produce necessarily connected decision regions. In this paper, we advance this important result by further developing the sufficient and necessary conditions under which the decision regions of a neural network are connected. We then apply our framework to overcome the limits of existing work and further study the capacity to learn connected regions of neural networks for a much wider class of activation functions including those widely used, namely ReLU, sigmoid, tanh, softlus, and exponential linear function.

1. Introduction

Deep learning has witnessed a transformed success in a diverse variety of application domains, notably computer vision (Krizhevsky et al., 2012), natural language processing (Bahdanau et al., 2014), speech recognition (Graves et al., 2013), and generative models (Kingma & Welling, 2013; Goodfellow et al., 2014). While these applied deep learning methods have hugely fueled by successful applications, important theoretical investigations are generally lacked behind. Theoretical studies tie hand-in-hand with practical aspects to help us with insights to train and tame deep learning models. Some important theoretical questions have been studied intensively in the literature, these include the representation power of neural networks with respect to their depth and width, the landscape of the loss surfaces of deep learning networks, and the capacity to learn connected regions in the input data space. The first question relates to the design of architectures for neural networks; the second question concerns the training aspect of deep learning models, while the last question has important implications in the study of the generation of adversarial samples.

The first important progress in the study of representation power of deep NNs is the universal approximation theorems (Cybenko, 1989; Hornik et al., 1989) which state that a feed-forward network with a single hidden layer containing a finite number of neurons can approximate continuous functions on compact subsets of $\mathbb{R}^d$, under mild assumptions on the activation function. Other subsequent works (Delalleau & Bengio, 2011; Eldan & Shamir, 2016; Safran & Shamir, 2017; Mhaskar & Poggio, 2016; Liang & Srikant, 2016; Yarotsky, 2017; Poggio et al., 2017) have been proposed to analyze the representation power of neural networks w.r.t their depth. In particular, it has been shown that there exist functions that can be computed efficiently by deep networks of linear or polynomial size but require exponential size for shallow networks. Last but not least, some recent works have studied the power of width efficiency (Lu et al., 2017; Hanin & Sellke, 2017). In particular, these works have indicated that neural networks with ReLU activation function have to be wide enough in order to have the universal approximation property as depth increases. More specifically, the authors prove that the class of continuous functions on a compact set cannot be arbitrarily well approximated by an arbitrarily deep network if the maximum width of the network is not larger than the input dimension $d$.

Regarding the second question on the landscape of the loss surfaces of deep learning networks, there have been several interesting results recently (Brutzkus & Globerson, 2017; Poggio & Liao, 2017; Rister & Rubin, 2017; Soudry & Hoffer, 2017). For some classes of networks it can be shown that the global optimum can be obtained efficiently. However, due to the requirement of knowledge about the data generating measure, or the strict specification of the neural network structure and optimization objective formulation (Gautier et al., 2016), these approaches are generally not practical (Janzamin et al., 2015; Soltanolkotabi, 2017). Another class of networks whose every local minimum is also a global minimum has
been shown to be deep linear networks (Baldi & Hornik, 1989; Kawaguchi, 2016). While this is a highly non-trivial result as the optimization problem is non-convex, deep linear networks are generally less preferable in practice since they are limited in linear function regime. In order to characterize the loss surface for general networks, an interesting approach was taken by (Choromanska et al., 2015). By randomizing the nonlinear part of a feedforward network with ReLU activation function and making some additional simplifying assumptions, the authors can map it to a certain spin glass model under which one can analyze analytically. In particular, the local minima are shown to be close to the global optimum and the number of bad local minima decreases quickly with the distance to the global optimum. Recently, the works of (Nguyen & Hein, 2017; 2018) have shown that for deep neural networks with a very wide layer, where the number of hidden units is larger than the number of training points, a large class of local minima is globally optimal, which generalizes the previous work of (Yu & Chen, 1995).

The theoretical question on the capacity of deep networks to learn connected decision regions is a particularly important one and has been recently addressed in (Nguyen et al., 2018). In particular, (Nguyen et al., 2018) has shown that for a feed-forward neural network with a pyramid architecture, the full-ranked weight matrices, and the strictly monotonically increasing continuous activation functions \( \sigma \) with \( \sigma(\mathbb{R}) = \mathbb{R} \) at each layer, the decision regions are connected. While this work has pioneered the preliminary results for this problem, its theoretical analysis only holds for a fairly narrow class of activation functions notably including the leaky ReLU, which is less used in practice. It is hence important to question the necessary and sufficient conditions under which a feedforward neural network’s decision regions are connected and if the theory can be extended for a much wider class of activation functions including those widely used in practice such as ReLU, sigmoid, tanh, softlus, and exponential linear function. Our goal in this paper is to advance the theories achieved in the previous work (Nguyen et al., 2018) by answering these questions. Specifically, we first propose the sufficient and necessary conditions for which a feedforward neural network’s decision regions are connected and then, base on these conditions to study when a feedforward neural network with the popular aforementioned activation functions can learn connected decision regions.

2. Related Background

We briefly introduce the convention used to describe feedforward neural networks, followed by the definition of a path-connected set and related properties.

2.1. Feedforward Neural Networks

We consider feedforward neural networks for the multi-class classification problem. Let us denote the number of classes by \( M \) (i.e., the class label \( y \in \{1, 2, \ldots, M\} \)) and the input dimension by \( d \) (i.e., the data sample \( x \in \mathbb{R}^d \)). Let us consider a feedforward neural network with \( L \) layers wherein the input layer is indexed by 0 and the output layer is indexed by \( L \). We further denote the width of layer \( k \) (i.e., \( 0 \leq k \leq L \)) by \( n_k \). For consistency, we enforce the constraints \( n_0 = d \) and \( n_L = M \). For each hidden layer \( k \) (i.e., \( 1 \leq k \leq L - 1 \)), we define the activation function for this layer as \( \sigma_k : \mathbb{R} \rightarrow \mathbb{R} \). We also define the feature map function over the layer \( k \) (\( 0 \leq k \leq L \)) as a function \( f_k : \mathbb{R}^d \rightarrow \mathbb{R}^{n_k} \), which computes for every input \( x \in \mathbb{R}^d \) a feature vector at layer \( k \) defined recursively as:

\[
f_k(x) = \begin{cases} 
    x & k = 0 \\
    \sigma_k(W_kf_{k-1}(x) + b_k) & 1 \leq k \leq L - 1 \\
    W_Lf_{L-1}(x) + b_L & k = L 
\end{cases}
\]

where \( W_k \in \mathbb{R}^{n_k \times n_{k-1}} \) is the weight matrix and \( b_k \in \mathbb{R}^{n_k} \) is the bias vector at the layer \( k \).

2.2. Activation Functions

We consider a range of the activation functions widely used in deep learning.

**Sigmoid function** The sigmoid function squashes its input into the range (0; 1):

\[
\text{sigmoid}(t) = \frac{1}{1 + \exp(-t)}
\]

**Tanh function** The tanh function squashes its input into the range (−1; 1):

\[
\text{tanh}(t) = \frac{\exp(-t) - \exp(t)}{\exp(-t) + \exp(t)}
\]

**ReLU function** The ReLU function squashes its input into the range \([0; +\infty)\):

\[
\text{ReLU}(t) = \max\{0; t\}
\]

**Leaky ReLU function** The leaky ReLU function squashes its input into the range \((−\infty; +\infty)\):

\[
\text{LeakyReLU}(t) = \max\{\alpha t; t\}
\]

where \( 0 < \alpha < 1 \).

**Softlus** The softlus function squashes its input into the range \((0; +\infty)\):

\[
\text{Softlus}(t) = \log(1 + \exp(t))
\]
Exponential linear function The exponential linear function squashes its input into the range $(-\alpha; +\infty)$: $$\text{ELU} (t) = \begin{cases} \alpha (\exp(t) - 1) & t < 0 \\ t & t \geq 0 \end{cases}$$ We note that except the ReLU function all other activation function are continuous bijections from $\mathbb{R}$ to their ranges.

2.3. Mapping Functions

Let $f : U \to V$ be a map from $U \subset \mathbb{R}^m$ to $V \subset \mathbb{R}^n$. We denote $\text{dom}(f) = U$ and $\text{range}(f) = f(U) = \{ v \mid v = f(u) \text{ for some } u \in U \}$. Given a subset $A \subset U$, the image $f(A)$ of this set via the map $f$ is defined as: $$f(A) = \{ v \mid v = f(u) \text{ for some } u \in A \} = \bigcup_{u \in A} \{ f(u) \}$$

**Definition 1. (Pre-image)** Given a map $f : U \to V$, the preimages of an element $v \in V$ and a subset $A \subset V$ via this map are defined as $$f^{-1}(v) = \{ u \in U \mid f(u) = v \}$$ $$f^{-1}(A) = \{ u \in U \mid f(u) \in A \}$$

**Proposition 2.** Let $f : U \to V$, $g : V \to T$ with $U \subset \mathbb{R}^m$, $V \subset \mathbb{R}^n$, $T \subset \mathbb{R}^p$, and $A \subset \mathbb{R}^p$. Then we have $$(g \circ f)^{-1}(A) = f^{-1} \left( g^{-1}(A \cap g(V)) \right)$$

2.4. Connectivity of Decision Regions

We briefly recap the definition and properties of path connectivity used in sequel development. We will also recall key theoretical results reported in (Nguyen et al., 2018).

**Definition 3. (Path-connected)** Consider $\mathbb{R}^m$ with the standard topology. A subset $A \subset \mathbb{R}^m$ is said to be path-connected if for every $u, v \in A$, there exists a continuous map $f$ from $[0; 1]$ to $A$, i.e., $f : [0; 1] \to A$ such that $f(0) = u$ and $f(1) = v$.

**Corollary 4.** If $g : U \to V$ is a continuous map and $A \subset U$ is a path-connected set then $g(A)$ is also a path-connected set.

**Corollary 5.** If $g : U \to V$ is a continuous bijection and $B \subset V$ is a path-connected set then $g^{-1}(B)$ is also a path-connected set.

With reference to the description of feedforward neural networks in Section 2.1, we now present the definition of decision region for each class whose connectivity is central to our theory.

**Definition 6. (Decision region)** Given a neural network with $L$ layers, the decision region of a given class $1 \leq m \leq M$, denoted by $C_m$, is defined as $$C_m = \{ x \in \mathbb{R}^d \mid (f_L)_m(x) > (f_L)_j(x), \forall j \neq m \}$$

We now recall the main results studied in (Nguyen et al., 2018).

**Theorem 7.** (Nguyen et al., 2018) Let the width of the layers of the feedforward neural network satisfy $d = n_0 \geq n_1 \geq n_2 \geq \cdots \geq n_{L-1}$ and let $\sigma_l : \mathbb{R} \to \mathbb{R}$ be continuous, strictly monotonically increasing activation function with $\sigma_l(\mathbb{R}) = \mathbb{R}$ for every layer $1 \leq l \leq L - 1$ and all the weight matrices $(W_l)_{i=1}^{d-1}$ have full rank. Then every decision region $C_m$ is an open connected subset of $\mathbb{R}^n$ for every $1 \leq m \leq M$.

3. Main Theoretical Results

3.1. Notations

We denote by $1 \in \mathbb{R}^n$ the vector of all 1, $1_k \in \mathbb{R}^n$ the one-hot vector with 1 at the $k$-th index and 0 at others, and 0 as the vector of all 0. Given a vector $u \in \mathbb{R}^n$ and $1 \leq i \leq j \leq n$, $u_{i:j}$ is defined as the sub vector $[u_k]_{i \leq k \leq j}$. Given two vectors $u, v \in \mathbb{R}^n$, the segment $[u, v]$, connecting $u$ and $v$ defined as $[u, v] = \{ x = (1 - t)u + tv \mid t \in [0; 1] \}$. A set $A \subset \mathbb{R}^n$ is said to be a convex set if the segment $[u, v] \subset A$ for every $u, v \in A$. We say that $u \leq v$ if only if $u_i \leq v_i$ for every $1 \leq i \leq n$; other operators, namely $>, <, <$, are defined in a similar element-wise manner. We define $\max \{ u, v \} = \{ \max \{ u_i, v_i \} \}_{i=1}^{n}$ and $\min \{ u, v \} = \{ \min \{ u_i, v_i \} \}_{i=1}^{n}$. We also define $\text{Rect}(u, v) = \{ x \in \mathbb{R}^n \mid \min \{ u, v \} \leq x \leq \max \{ u, v \} \}$, $\text{Rect}(u) = \{ x \in \mathbb{R}^n \mid u \leq x \}$ and $\text{Rect}(u, v) = \{ x \in \mathbb{R}^n \mid \min \{ u, v \} < x < \max \{ u, v \} \}$, $\text{Rect}(u) = \{ x \in \mathbb{R}^n \mid u < x \}$.

It is well-known that for a finite-dimensional normed space $\mathbb{R}^n$, all norms are equivalent (See Theorem 2.2.16 in (Hsing & Eubank, 2015)), hence inducing the same topology. We use the standard topology on $\mathbb{R}^n$ to imply this identical topology which can be induced by any norm in this space. Consider $\mathbb{R}^n$ with the standard topology and with the norm $\| \cdot \|$. An open ball with the center $x$ and the radius $r > 0$ is defined as $B(x, r) = \{ y \in \mathbb{R}^n \mid \| y - x \| < r \}$. Based on the standard topology on $\mathbb{R}^n$, we define the closure set $A$ by $\text{cl}(A)$, which is the smallest closed super set of $A$ and the interior set of $A$ by $\text{int}(A)$, which is the largest open subset of $A$.

3.2. Theoretical Results

In this section, we present our main theory for the path connectivity of decision regions induced by a feedforward neural network. We start this section with the definition of the piecewise connectivity.

**Definition 8. (Piecewise-connected)** Consider $\mathbb{R}^m$ with the standard topology. A subset $A \subset \mathbb{R}^m$ is said to be a piecewise-connected set if for every $u, v \in A$, there exists
a sequence of elements $x_1 = u, x_2, \ldots, x_n = v$ in $A$ such that the segments $[x_i, x_{i+1}] \subset A$ for every $1 \leq i \leq n - 1$.

In the following theorem, we study the theoretical relationship between path connectivity and piecewise connectivity. It turns out that in a standard topology over $\mathbb{R}^m$, these two concepts of connectivity are equivalent. To prove this central theorem, we need the following lemmas.

**Lemma 9.** Let $B_1 = B(x_1, r_1)$ and $B_2 = B(x_2, r_2)$ be two joint sets (i.e., $B_1 \cap B_2 \neq \emptyset$). Then the segment $[x_1, x_2] \subset B_1 \cup B_2$.

**Proof.** Let $x = (1 - t)x_1 + tx_2$ with $0 \leq t \leq 1$. We have $\|x - x_1\| = t\|x_1 - x_2\|$ and $\|x - x_2\| = (1 - t)\|x_1 - x_2\|$. Then

$$\|x - x_1\| + \|x - x_2\| = \|x_1 - x_2\| < r_1 + r_2$$

Hence, either $\|x - x_1\|$ or $\|x - x_2\|$ is less than $r_1$ or $r_2$ respectively which implies $x \in B_1 \cup B_2$. $\square$

**Lemma 10.** Let a path-connected subset $A \subset \mathbb{R}^m, u, v \in A$, and a continuous function $f: [0; 1] \to A$ with $f(0) = u, f(1) = v$. Let $P, Q$ be two open sets such that $u \in P, v \in Q, f([0; 1]) \subset P \cup Q$. Then, $P \cap Q \neq \emptyset$.

**Proof.** Since $P, Q$ are two open sets, $f^{-1}(P)$ and $f^{-1}(Q)$ are also open in $[0; 1]$ and these two sets are non-empty due to $0 \in f^{-1}(P)$ and $1 \in f^{-1}(Q)$. Moreover, $f^{-1}(P) \cap f^{-1}(Q) = [0; 1]$. This means that we can find two non-empty open sets $f^{-1}(P)$ and $f^{-1}(Q)$ such that $f^{-1}(P) \cap f^{-1}(Q) = [0; 1]$. Therefore, $f^{-1}(P) \cap f^{-1}(Q) \neq \emptyset$ because otherwise $[0; 1]$ is not connected. Finally, we obtain $P \cap Q \neq \emptyset$. $\square$

**Theorem 11.** Consider $\mathbb{R}^m$ with the standard topology. An open subset $A \subset \mathbb{R}^m$ is path-connected if only if it is piecewise-connected.

**Proof.** We prove two ways of this theorem.

Assume that $A$ is piecewise-connected. Given two elements $u, v$ in $A$, there exists a sequence of elements $x_1 = u, x_2, \ldots, x_n = v$ in $A$ such that the segments $[x_i, x_{i+1}] \subset A$ for every $1 \leq i \leq n - 1$. Let us consider the following function that maps from $[0; 1]$ to $A$:

$$f(t) = \sum_{i=0}^{n-1} 1_{t \in \left[\frac{i}{n}, \frac{i+1}{n}\right]}(t) [(i + 1 - nt) x_1 + (nt - i) x_{i+1}]$$

where $1_S(t)$ returns 1 if the statement $S$ is true and 0 otherwise.

This function is continuous, $f(0) = x_1 = u, f(1) = x_n = v$, and $f([0; 1]) \subset A$. This implies that $A$ is also path-connected.

We now assume that $A$ is path-connected. Given two elements $u, v$ in $A$, there exists a continuous function mapping from $[0; 1]$ to $A$ such that the arc $f([0; 1])$ connecting $u, v$ lies in $A$. Since $[0; 1]$ is a compact set and $f$ is continuous, the arc $f([0; 1])$ is a compact set in $\mathbb{R}^m$. $A$ is an open set, hence for each $x \in A$ there exists an open ball $B(x, r_x) \subset A$. We consider $I = \{x \mid B(x, r_x) \cap f([0; 1]) \neq \emptyset\}$. It is obvious that $f([0; 1]) \subset I$, hence the collection $\{B(x, r_x) \mid x \in I\}$ is an open coverage of $f([0; 1])$. From the compactness of $f([0; 1])$, there exists an finite open coverage $\{B(x, r_x) \mid x \in J\}$ where $J \subset I$ is finite. Without loss of generality, we assume that $u, v \in J$ because otherwise we can extend $J$. We now construct a graph $G = (V, E)$ where the set of vertices $V \subset J$ and the set of edges $E$ are all initialized by $\emptyset$ and gradually conducted as follows. We first set $V = \{x_1\}$ where $x_1 = u$. We then set $P = B(x_1, r_{x_1})$ and $Q = \bigcup_{x \in J \setminus V} B(x, r_x)$. This is obvious, $P, Q$ are two open sets satisfying the conditions in Lemma 10, hence $P \cap Q \neq \emptyset$ which implies there exists $x_2 \in J \setminus V$ such that $P \cap B(x_2, r_{x_2}) \neq \emptyset$. We then add $x_2$ to $V$ and also the edge $x_1 x_2$ to $E$. In general, at each step we define $P = \bigcup_{x \in V} B(x, r_x)$ and $Q = \bigcup_{x \in J \setminus V} B(x, r_x)$. Two open sets $P, Q$ obviously satisfy the conditions in Lemma 10, hence $P \cap Q \neq \emptyset$. We now consider two cases:

- $B(x_1, r_{x_1}) \cap B(v, r_v) \neq \emptyset$ for some $x_1 \in V$: we set $z_{n+1} = v$ where $n = |V|$, then add $z_{n+1}$ to $V$ as well as the edge $x_1 z_{n+1}$ to $E$, and stop the algorithm to construct $G = (V, E)$.
- $B(x_1, r_{x_1}) \cap B(x_2, r_{x_2}) \neq \emptyset$ for some $x_1, x_2 \in V \setminus J$: we set $z_{n+1} = x_2$ where $n = |V|$, then add $z_{n+1}$ to $V$ as well as the edge $x_1 z_{n+1}$ to $E$, and continue the algorithm to construct $G = (V, E)$.

It is worth noting that the graph $G = (V, E)$ constructing using the above algorithm is always a connected tree. In addition, due to the finiteness of $J$, the aforementioned algorithm must be halted and ends with $v \in V$. We now consider the path $u = z_1 = z_{i_0}, z_{i_1}, \ldots, z_{i_{k-1}}, z_{i_k} = v$ connecting $u$ and $v$ in $G$. By way of constructing this graph, we have $B(z_{j_1}, r_{z_{j_1}}) \cap B(z_{j_1+1}, r_{z_{j_1+1}}) \neq \emptyset$ for $j = 0, 2, \ldots, k - 1$. Using Lemma 9, we obtain $z_{j_1}, z_{j_1+1} \in B(z_{j_1}, r_{z_{j_1+1}}) \cup B(z_{j_1+1}, r_{z_{j_1+1}}) \subset A$. This concludes that $A$ is a path-connected set.

**Lemma 12.** Let $h : U \to V$ be an onto affine map with $U \subset \mathbb{R}^m, V \subset \mathbb{R}^n$, and $h(u) = Wu + b$. Let $B \subset V$ be an open path-connected subset of $V$. Then $A = h^{-1}(B)$ is an open path-connected subset of $U$.

**Proof.** Let $u_1, u_2 \in A$ then $v_1 = h(u_1) \in B$ and $v_2 = h(u_2) \in B$. Due to the path and also piece-
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wista connectivity of the open set $B$, there exists $y_i = v_1, y_2, \ldots, y_{n-1}, y_n = v_2$ such that $[y_i, y_{i+1}] \subset B$ for $1 \leq i \leq n-1$. Since $h$ is an onto linear map, there exists $x_i \in U$ such that $h(x_i) = y_i$ for every $1 \leq i \leq n$. In addition, the linearity of $h$ gives us $h([x_{i}, x_{i+1}]) = [h(x_{i}), h(x_{i+1})] = [y_i, y_{i+1}] \subset B, \forall i$. This follows that $[x_i, x_{i+1}] \subset h^{-1}(B) = A, \forall i$. This concludes $A$ is an open path (piecewise) connected set.

**Lemma 13.** Let $h : U \to V$ be an onto affine map with $U \subset \mathbb{R}^m$, $V \subset \mathbb{R}^n$, and $h(u) = Wu + b$. Let $B \subset V$ be a convex subset of $V$. Then $h^{-1}(B)$ is a convex subset of $U$.

**Proof.** Let $u_1, u_2 \in A$ then $v_1 = h(u_1) \in B$ and $v_2 = h(u_2) \in B$. Due to the convexity of $B$, the segment $[v_1, v_2] \subset B$. In addition, the linearity of $h$ gives us $h([u_1, u_2]) = h(u_1) + h(u_2) = [v_1, v_2] \subset B$. This follows that $[u_1, u_2] \subset h^{-1}(B) = A$. This concludes $A$ is a convex set.

**Lemma 14.** Let $h : U \to V$ be an affine map with $U \subset \mathbb{R}^m$, $V \subset \mathbb{R}^n$, and $h(u) = Wu + b$. Let $A \subset U$ be a convex subset of $A$. Then $B = h(A) \subset V$ is a convex subset of $B$.

**Proof.** Let $v_1 = h(u_1) \in B$ and $v_2 = h(u_2) \in B$ where $u_1, u_2 \in A$. From the convexity of $A$, the segment $[u_1, u_2] \subset A$. The linearity of $h$ gives us $v_1, v_2 \in h([u_1, u_2]) = [h(u_1), h(u_2)] = [v_1, v_2] \subset B$. This follows that $B$ is convex.

**Lemma 15.** Let $g : U \to V$ be an onto continuous map with $U \subset \mathbb{R}^m$, $V \subset \mathbb{R}^n$ and $B \subset V$ be a subset of $V$. If $B$ is not path-connected, $A = g^{-1}(B)$ is not path-connected too.

**Proof.** This is trivial from the fact that if $A$ is path-connected then $B = g(A)$ is also path-connected.

**Lemma 16.** Define $\hat{\sigma} : \mathbb{R}^n \to \mathbb{R}^n$ as $\hat{\sigma}(x) = [\sigma(x_1) \ldots \sigma(x_n)]^T$ where $x = [x_1 \ldots x_n]^T$. Let $V \subset \mathbb{R}^n$ be a path-connected set. Then $U = \hat{\sigma}^{-1}(V)$ is also a path-connected set.

**Proof.** This is trivial from the fact that $\hat{\sigma}^{-1} : V \to U$ is a continuous bijection map and $V$ is path-connected.

**Lemma 17.** Let $g : U \to V$ be a continuous map with $U \subset \mathbb{R}^m$, $V \subset \mathbb{R}^n$. Let $A \subset B \subset U$ such that $cl(A) = B$ and $g(B)$ is closed, then $g(A) \subset g(B) \subset V$ and $cl(g(A)) = g(B)$.

**Proof.** We first have $g(A) \subset g(B) \subset V$, hence $cl(g(A)) \subset cl(g(B)) = g(B)$. Now let $v = g(u) \in g(B)$ with $u \in B$, since $cl(A) = B$, there exists a sequence $\{u_n\}_{n=1}^{\infty} \subset A$ and $\lim_{n \to \infty} u_n = u$. From the continuity of $g$, we obtain $\lim_{n \to \infty} g(u_n) = g(u) = v$. This follows that $v \in cl(g(A))$ or $g(B) \subset cl(g(A))$.

We are now in a position to state the necessary and sufficient conditions under which decision regions for classes are path-connected (cf. Theorem 18). To support the theorem stated, we further introduce the set $D_m$ defined as

$$D_m = \{ o \in \mathbb{R}^M | o_m > o_j, \forall j \neq m \}$$

It is clear that $D_m$ is an open convex set since formed by the intersection of $M$ half-spaces $H_j = \{ o \in \mathbb{R}^M | o_m > o_j \}$.

**Theorem 18.** For every $1 \leq m \leq M$ the decision region $C_m$ is an open path-connected set if only if $f_L (\mathbb{R}^d) \cap D_m$ is an open path-connected set provided that $f_L (x)$ is a feedforward neural network and the activation functions $\sigma_k, 1 \leq k \leq L - 1$ used in this network are continuous bijections (i.e., $\sigma_k$ can be the sigmoid, tanh, leaky ReLU, sofplus, and exponential linear activation functions).

**Proof.** While $C_m$ and $f_L (\mathbb{R}^d) \cap D_m$ are open sets, we prove that if $f_L (\mathbb{R}^d) \cap D_m$ is a path-connected set, so is $C_m$ and if $f_L (\mathbb{R}^d) \cap D_m$ is not a path-connected set, so nor is $C_m$.

Let us denote $A_1 = h_1(C_m)$ where $h_1(\cdot) = W_1 \cdot + b_1$ and $B_1 = \hat{\sigma}_1(A_1) = f_1(C_m)$. The sets $A_2, B_2$ are defined based on $B_1$ as $A_2 = h_2(B_1)$ where $h_2(\cdot) = W_2 \cdot + b_2$ and $B_2 = \hat{\sigma}_2(A_2)$. In general, the sets $A_k, B_k, 1 \leq k \leq L - 1$ are defined recursively as $A_k = h_k(B_{k-1})$ where $h_k(\cdot) = W_k \cdot + b_k$ and $B_k = \hat{\sigma}_k(A_k)$. Finally, we define $A_L = h_L(B_{L-1})$ where $h_L(\cdot) = W_L \cdot + b_L$. We now prove that $A_L = f_L (\mathbb{R}^d) \cap D_m$, hence $f_L (x)$ is an onto map from $C_m$ to $A_L$. In fact, taking any $o \in f_L (\mathbb{R}^d) \cap D_m$, there exists $x \in \mathbb{R}^d$ such that $f_L (x) = o$ and it is also obvious that $x \in C_m$ from the definition of $D_m$.

Since $B_{L-1} = h_{L-1}^{-1}(A_L)$ and $h_L(\cdot)$ is an affine map, $B_{L-1}$ is an open path-connected set. Using the fact that $A_{L-1} = \hat{\sigma}_{L-1}^{-1}(B_{L-1})$ and $\sigma_{L-1}$ is a continuous bijection, $A_{L-1}$ is also an open path-connected set (Lemma 16). Using the fact that $A_{L-2} = h_{L-2}(B_{L-2})$ and $A_{L-2}$ is an affine map, we reach $B_{L-2}$ is an open path-connected set. Using the fact that $A_{L-2} = \hat{\sigma}_{L-2}^{-1}(B_{L-2})$ and $\sigma_{L-2}$ is a continuous bijection, $A_{L-2}$ is also an open path-connected set (Lemma 16). Repeating this argument backward the layers of the neural network, we obtain $A_1, B_1$ are open path-connected sets. Finally from $A_1 = h_1(C_m)$ and $h_1(\cdot)$ is an affine map, we reach the conclusion that $C_m$ is an open path-connected subset of $\mathbb{R}^d$.

The converse is trivial from the fact that $f_L (C_m) = A_L = f_L (\mathbb{R}^d) \cap D_m$ and $f_L (\cdot)$ is a continuous map, hence if
\[f_L (\mathbb{R}^d) \cap D_m \text{ is not a path-connected set, } C_m \text{ is also not a path-connected set (thanks to Lemma 15).} \]

**Lemma 19.** If \(cl (B) \) is a convex polyhedron, then \(B \) is a path-connected set.

**Proof.** If \(B = \emptyset \), then it is path-connected. Now assume that \(B \neq \emptyset \), let \(w \in int (B) \), then there exists \(B (w, r) \subset B \). Consider any \(u, v \in B \). We prove that \([w, u] \) and \([w, v] \) are subsets of \(B \) to reach the conclusion. In fact, we first have \([u, a] \subset cl (B) \) for any \(a \in B (w, r) \), hence \([u, w] \setminus \{u\} \) is a subset of \(int (cl (B)) \). Since \(cl (B) \) is a polyhedron, we obtain \(int (cl (B)) \subset B \). Therefore, we reach \([w, u] \subset B \). Similarly, we obtain \([w, v] \subset B \). \[\square\]

**Lemma.** If \(B_1 \) and \(B_2 \) are two polyhedrons, then \(cl (B_1 \cap B_2) = cl (B_1) \cap cl (B_2) \).

**Proof.** Let \(B_1 = \{u \mid W_1 u < b_1, W_2 u = b_2\} \) and \(B_2 = \{u \mid W_3 u < b_3, W_4 u = b_4\} \). We then have:

\[cl (B_1 \cap B_2) = cl (B_1) \cap cl (B_2) \]

\[\{u \mid W_1 u < b_1, W_2 u = b_2, W_3 u < b_3, W_4 u = b_4\} \]

**Lemma.** Let \(B = \{u \mid M u \leq m, N u = n\} \) be a closed polyhedron and \(h (u) = u + b \) be an affine map, then \(h (B) \) is a closed polyhedron.

**Proof.** We consider

\[C = \{(u, v) \mid M u \leq m, N u = n, v = u + b\} \]

then \(C \) is a closed polyhedron.

We now remark that \(h (B) = \pi_v (C) \) where \(\pi_v (u, v) = v \) is the projection map. This leads to the conclusion. \[\square\]

**Theorem 18** sheds light on devising neural networks whose decision regions are connected. Based on this theorem, we can formulate a sufficient condition for a given neural network being able to learn connected decision regions stated in Corollary 20.

**Corollary 20.** Consider a feedforward neural network with \(L \) layers and \(A = f_{L-1} (\mathbb{R}^d) \). If either \(A \) is a convex set or \(cl (A) \) is a polyhedron, then \(C_m \) is an open path-connected set for every \(1 \leq m \leq M \).

**Proof.** Let \(h_L (\cdot) = W_L \cdot + b_L \) be the affine map at the last layer. Assume that \(A \) is convex, then \(f_L (\mathbb{R}^d) = h_L (f_{L-1} (\mathbb{R}^d)) \). Since \(h_L (A) \) is a convex subset of \(\mathbb{R}^M \) (thanks to Lemma 14), this follows that \(f_L (\mathbb{R}^d) \cap D_m \) is a convex set for every \(1 \leq m \leq M \) due to the convexity of \(D_m \). Theorem 18 can be applied to reach the conclusion since \(f_L (\mathbb{R}^d) \cap D_m \) is a path-connected set for every \(m \). We now assume that \(cl (A) \) is a polyhedron. This follows that \(h_L (cl (A)) \) is a closed polyhedron since \(h_L \) is an affine map. Referring to Lemma 17, we obtain \(cl (h_L (A)) = h_L (cl (A)) \), which is a polyhedron. Since \(D_m \) is also a polyhedron, we obtain \(cl (h_L (A) \cap D_m) = cl (h_L (A)) \cap cl (D_m) \) is also a polyhedron. By applying Lemma 19, we arrive \(h_L (A) \cap D_m = f_L (\mathbb{R}^d) \cap D_m \) is a path-connected set. \[\square\]

To see the usefulness of our new result in Corollary 20, we use it to provide an alternative proof for the result stated in (Nguyen et al., 2018) (Theorem 3.10 in that paper). Compared original proof, our alternative proof does not require monotonically increasing property. Corollary 20 also becomes extremely useful in our later theoretical development to study of decision regions for a general continuous bijective activation function (e.g., the leaky ReLU, ELU, softflus, sigmoid, and tanh activation functions) which was not possible to develop under the framework of (Nguyen et al., 2018).

**Theorem 21.** (first stated in (Nguyen et al., 2018) and being re-proved here) Let the width of the layers of the feedforward neural network satisfy \(d = n_0 \geq n_1 \geq n_2 \geq \cdots \geq n_{L-1} \). Let \(\sigma : \mathbb{R} \to \mathbb{R} \) be bijective continuous activation function for every layer \(1 \leq l \leq L - 1 \) and all the weight matrices \(W_l \) have full rank. If \(\sigma_1 (\mathbb{R}) = \mathbb{R} \) for every layer \(1 \leq l \leq L - 1 \) then every decision region \(C_m \) (i.e., \(1 \leq m \leq M \)) is an open connected subset of \(\mathbb{R}^d \).

**Proof.** Let us denote \(A_l = f_l (\mathbb{R}^d) \), \(B_l = \sigma_l (A_l) \), and \(h_l (\cdot) = W_l \cdot + b_l \) (i.e., the linear map at the layer \(l \)) for \(1 \leq l \leq L - 1 \). It is obvious that \(A_{l+1} = h_{l+1} (B_l) \) for \(0 \leq l \leq L - 2 \) with the assumption that \(B_0 = \mathbb{R}^d \).

The facts \(A_1 = h_1 (\mathbb{R}^d) \) and \(W_1 \) is full rank gives us \(A_1 = \mathbb{R}^{n_1} \). The facts \(B_1 = \sigma_1 (A_1) \) and \(\sigma_1 \) is a bijective continuous map with \(\sigma_1 (\mathbb{R}) = \mathbb{R} \) gives us \(B_1 = \mathbb{R}^{n_1} \).

Similarly, we obtain \(A_2 = B_2 = \mathbb{R}^{n_2} \) and finally \(A_{L-1} = B_{L-1} = \mathbb{R}^{n_{L-1}} \). Note that \(f_{L-1} (\mathbb{R}^d) = B_{L-1} = \mathbb{R}^{n_{L-1}} \) certainly satisfies the condition in Corollary 20, we reach the conclusion. \[\square\]

Given a full rank matrix \(W \in \mathbb{R}^{n \times m} \) with \(n \leq m \), there exists \(n \) linearly independent columns, e.g., \(W_1, \ldots, W_n \), of \(W \). In other words, the matrix \(W^1 = [W_1 \ W_2 \ldots W_n] \in \mathbb{R}^{n \times n} \) formed by these columns has rank \(n \) and is invertible, while the matrix \(W^2 \) formed by the rest columns is in \(\mathbb{R}^{n \times (m-n)} \). Here we note that the columns in \(W^1 \) do not need to be consecutive. However, for the sake of simplicity, without loss of generalization we assume that they are in a row. Furthermore, since each column in \(W^2 \) can be represented as a linear combination of those in \(W^1 \), there exists a matrix \(U \in \mathbb{R}^{m \times (m-n)} \) such that \(W^2 = W^1 U \).
When Can Neural Networks Learn Connected Decision Regions?

We next study under which conditions an affine transformation transform $\text{Rect}(u_1, u_2)$ to $\text{Rect}(v_1, v_2)$ or $\text{Rect}(u)$ to $\text{Rect}(v)$.

**Corollary 22.** Let $h : \mathbb{R}^m \to \mathbb{R}^n$ be an affine map with $h(u) = W u + b$ where $W \in \mathbb{R}^{n \times m}$ is a full rank matrix $(m \geq n)$. Let $W = [W^1 W^2]$ wherein $W^1 \in \mathbb{R}^{n \times n}$ and $W^2 \in \mathbb{R}^{n \times (m-n)}$ are defined as above. If $W$ and $V$ are two non-negative matrices with $V = (W^1)^{-1}$, the image of $\text{Rect}(u) \subset \mathbb{R}^m$ is $\text{Rect}(v) \subset \mathbb{R}^n$ with $v = h(u)$.

**Proof.** Let $y \geq v = h(u) = W u + b$. Let $a^1 = V(y-v) \in \mathbb{R}^n$, $a^2 = 0_{m-n} \in \mathbb{R}^{m-n}$, and $a = [a^1 a^2]^T$. Let $x = u + a \in \mathbb{R}^m$. We then have

$$h(x) = W u + W a + b = W^1 a^1 + W^2 a^2 + v = W^1 V (y-v) + v = y$$

In addition, since $V \geq 0$ and $y - v \geq 0$, we obtain $a^1 \geq 0$ and hence $a \geq 0$. This follows that $x \geq u$ and $x \in \text{Rect}(u)$. Thus, we reach the conclusion that $\text{Rect}(v) \subset h(\text{Rect}(u))$. Moreover, let $x \in \text{Rect}(u)$. Since $W \geq 0$, we have

$$W x + b \geq W u + b = v$$

$$y = h(x) \geq h(u) = v$$

Therefore, $y \in \text{Rect}(v)$ and this implies $h(\text{Rect}(u)) \subset \text{Rect}(v)$. Finally, we arrive $h(\text{Rect}(u)) = \text{Rect}(v)$. 

**Corollary 23.** Let $h : \mathbb{R}^m \to \mathbb{R}^n$ be an affine map with $h(u) = W u + b$ where $W \in \mathbb{R}^{n \times m}$ is a full rank matrix $(m \geq n)$. Let $W = [W^1 W^2]$ and $W^2 = W^1 U$ wherein $W^1 \in \mathbb{R}^{n \times n}$, $W^2 \in \mathbb{R}^{n \times (m-n)}$, and $U \in \mathbb{R}^{m \times (m-n)}$ are defined as above. If $W$ and $V$ are two non-negative matrices, and $U [\Delta u_{i1}]_{i=1}^{m+n} \leq 0$ where $V = (W^1)^{-1}$, $u \leq u_2$, $\Delta u = u_2 - u_1$, the image of $\text{Rect}(u_1, u_2) \subset \mathbb{R}^m$ with $u_1 \leq u_2$ is $\text{Rect}(v_1, v_2) \subset \mathbb{R}^n$ with $v_1 \leq v_2$ where $v_1 = h(u_1)$ and $v_2 = h(u_2)$.

**Proof.** It is trivial that $v_1 \leq v_2$ from the facts $u_1 \leq u_2$ and $W \geq 0$. Given $u \in \text{Rect}(u_1, u_2)$, hence $u_1 \leq u \leq u_2$, it is obvious that $h(u_1) \leq h(u) \leq h(u_2)$ or $v_1 \leq h(u) \leq v_2$. This follows that $h(u) \in \text{Rect}(v_1, v_2)$, hence $h(\text{Rect}(u_1, u_2)) \subset \text{Rect}(v_1, v_2)$.

Let $1_i \in \mathbb{R}^n$ be the one-hot vector with the only 1 at the $i$-th position. Let $v \in \text{Rect}(v_1, v_2)$ which can be represented as:

$$v = [\lambda_i (v_{2,i} - v_{1,i})]_{i=1,...,n}^T + v_1 = \sum_{i=1}^{n} 1_i \lambda_i (v_{2,i} - v_{1,i}) + v_1,$$

where $0 \leq \lambda_i \leq 1$, $\forall i$.

Let us denote

$$u = \left[ \sum_{i=1}^{n} V_i \lambda_i (u_2 - u_1) \right]_{[m-n]}^T + u_1$$

where $V_i$ points out the $i$-th column of the matrix $V$, and $\lambda_i$ points out the $i$-th row of the matrix $V$. We now verify that $u \in \text{Rect}(u_1, u_2)$ or equivalently $u_1 \leq u \leq u_2$. Since $u_1 \leq u_2$, $W \geq 0$, and $V \geq 0$, it is obvious that $u_1 \leq u$. We further derive as follows:

$$\sum_{i=1}^{n} V_i \lambda_i (u_2 - u_1) \leq \sum_{i=1}^{n} V_i \lambda_i (u_2 - u_1) = V W \Delta u = V [W^1 W^2] \Delta u = \Delta u_{1:n+1:m} \leq \Delta u_{1:n}$$

Therefore, we obtain

$$u \leq [\Delta u_{1:n} 0_{m-n}]^T + u_1 \leq u_2$$

We now prove that $h(u) = v$. Indeed, we have

$$h(u) = W u + b = W \left[ \sum_{i=1}^{n} V_i \lambda_i (u_2 - u_1) \right]_{[m-n]}^T + W u_1 + b$$

$$= \sum_{i=1}^{n} V_i \lambda_i (u_2 - u_1) + v_1$$

Here we note that since $W^1 V = \mathbb{I}_n$, we have $W^1 V_i \lambda_i = 1_i$. Putting all-together, we have $h(u) = v$ with $u \in \text{Rect}(u_1, u_2)$ and this implies $\text{Rect}(v_1, v_2) \subset h(\text{Rect}(u_1, u_2))$. Finally, we reach the conclusion of $h(\text{Rect}(u_1, u_2)) = \text{Rect}(v_1, v_2)$. 

The matrix $W$ in Corollaries 22 and 23 is constructed based on the non-negative matrix $W^1$ whose inverse $V$ is also a non-negative matrix. This class of matrices, known as non-negative monomial matrix, has been studied in (Ding & Rhee, 2014) wherein it has been proven that $W^1$ is a non-negative monomial matrix if only if it can be
factorized as the multiplication of a non-negative diagonal matrix $D$ and a permutation matrix $P$, i.e., $W^1 = DP$. Based on the matrix $W^1$, we can flexibly construct the matrix $W^2$ satisfying the constraints in Corollaries 22 and 23. We now recruit Corollaries 22 and 23 as building blocks for Theorem 24 wherein we address the question under which conditions a feedforward neural network with the sigmoid, tanh, softplus, and ELU activation functions has connected decision regions.

**Theorem 24.** Let the width of the layers of the feedforward neural network satisfy $d = n_0 \geq n_1 \geq n_2 \geq \cdots \geq n_{L-1}$. Let $\sigma_i : \mathbb{R} \to \mathbb{R}$ be bijective continuous activation functions for every layer $1 \leq l \leq L - 1$, all the weight matrices $(W_l)_{i=1}^{n_l}$ have full rank.

i) If $\lim_{t \to +\infty} \sigma_i(t) = \alpha_1$, finite, $\lim_{t \to +\infty} \sigma_i(t) = +\infty$, $W_1$ and $V$ are two non-negative matrices wherein $V_1 = (W_1)^{-1}$ in which $W_1$ is defined from $W_l$ as above for every $2 \leq l \leq L$ then every decision region $C_m$ (i.e., $1 \leq m \leq M$) is an open path-connected subset of $\mathbb{R}^d$.

ii) If $\lim_{t \to +\infty} \sigma_i(t) = \alpha_1$, finite, $\lim_{t \to +\infty} \sigma_i(t) = +\infty$, $W_1$ and $V$ are two non-negative matrices, and $U_i [\Delta u_i]_{i=n_{i+1}}^{n_i+1} \leq 0$ where $\Delta u_i = u_i - u_i^1, u_i^1 = \sigma_i(W_iu_i^{-1} + b_i), u_i^2 = u_i(\sigma_i(W_iu_i^{-1} + b_i) + \sigma_i(W_iu_i^{-1} + b_i))$ with $u_i = [a_1]_{n_1}, u_i^1 = [a_2]_{n_1},$ and $V_i = (W_i)^{-1}$, $W_2 = W_1^1U_l$ in which $W_1$ and $W_2$ are defined from $W_1$ as above for every $2 \leq l \leq L$ then every decision region $C_m$ (i.e., $1 \leq m \leq M$) is an open path-connected subset of $\mathbb{R}^d$.

**Proof.** Let us denote $A_l = f_l(\mathbb{R}^d)$, $B_{l+1} = h_{l+1}(A_l)$ with $h_l(\cdot) = W_l \cdot + b_l$ (i.e., the affine map at the layer $l$) for $0 \leq l \leq L - 1$. It is obvious that $A_l = \sigma_l(B_l)$ for $1 \leq l \leq L - 1$. Since the matrix $W_1$ is full-ranked, $B_l = h_l(A_0) = h_l(\mathbb{R}^d) = \mathbb{R}^d$.

i) This follows that $A_1 = \sigma_1(B_1) = \sigma_1(\mathbb{R}^d) = (a_1, +\infty)^{n_1} = \text{Rect}(u^1)$ where $u^1 = [a_1]_{n_1}$. Using the facts that $W_2 \geq 0, V_2 \geq 0$ where $V_2 = (W_2)^{-1}$, Corollary 22 gives us $h_1(\text{Rect}(u^1)) = \text{Rect}(v)$ where $v = h_2(u^1)$. Using the facts that $\text{cl}(A_1) = \text{Rect}(u^1)$ and $h_1(\text{Rect}(u^1)) = \text{Rect}(u_1, u_2)$ and $h_1(\text{Rect}(u_2, u_2)) = \text{Rect}(v_1, v_2)$ is closed, Corollary 17 gives us $\text{cl}(B_2) = \text{Rect}(v_1, v_2)$, hence $B_2 \supset \text{Rect}(v_1, v_2)$. Since $A_2 = \sigma_2(B_2)$, we obtain $\text{cl}(A_2) = \text{Rect}(u_2^2, u_2^2)$. Using the same argument forward the network, we obtain $\text{cl}(A_{L-1}) = \text{Rect}(u_1, u_2^L)$ (i.e., a polyhedron), which concludes this proof (thanks to Corollary 20).

ii) This follows that $A_1 = \sigma_1(B_1) = \sigma_1(\mathbb{R}^d) = (a_1, a_2)^{n_1} = \text{Rect}(u_1, u_2)$ where $u_1 = [a_1]_{n_1}$ and $u_2 = [a_2]_{n_1}$. Using the facts that $W_2 \geq 0$, and $U_i [\Delta u_i]_{i=n_{i+1}}^{n_i+1} \leq 0$ where $V_2 = (W_2)^{-1}$, Corollary 23 gives us $h_1(\text{Rect}(v_1, v_2)) = \text{Rect}(v_1, v_2)$ where $v_1 = h_2(u_1)$ and $v_2 = h_2(u_2)$. Using the facts that $\text{cl}(A_1) = \text{Rect}(u_1, u_2)$ and $h_1(\text{Rect}(u_1, u_2)) = \text{Rect}(v_1, v_2)$ is closed, Corollary 17 gives us $\text{cl}(B_2) = \text{Rect}(v_1, v_2)$, hence $B_2 \supset \text{Rect}(v_1, v_2)$. Since $A_2 = \sigma_2(B_2)$, we obtain $\text{cl}(A_2) = \text{Rect}(u_2, u_2)$. Using the same argument forward the network, we obtain $\text{cl}(A_{L-1}) = \text{Rect}(u_1, u_2^L)$ (i.e., a polyhedron), which concludes this proof (thanks to Corollary 20).

It is worth noting that Theorem 24 can be applied to all bijective continuous activation functions including the leaky ReLU, ELU, softplus, sigmoid, and tanh activation functions. However, this cannot be applied to the ReLU activation function, which is one of the most widely used activation functions. The reason is that this activation function is not bijective. In what follows, we study the capacity to learn path-connected regions of a feed-forward neural net with the ReLU activation function.

**Corollary 25.** Let $h : \mathbb{R}^m \to \mathbb{R}^n$ be an affine map with $h(u) = Wu + b$ where $W \in \mathbb{R}^{n \times m}$ is a full rank matrix. If $V$ is a non-negative matrix and $Vb \leq 0$ where $V = (W_1)^{-1}$ with $W_1, W_2$ to be defined as above, we have $\text{Rect}(0_m) \subset h(\text{Rect}(0_m))$.

**Proof.** Let $v = [a_1 \cdots a_n]^T \in (\text{Rect}(0_n) \setminus \{0_n\})$. Let $v_i = V(1_i - \sum_{i=1}^n a_i) = V1_i - \sum_{i=1}^n a_i b_i \geq 0 \in \mathbb{R}^n$ where $1_i$ is the one-hot vector with 1 at the $i$-th index for $1 \leq i \leq n$. We further define $u_i = [v_i^T 0_{m-n}^T]^T$ and $u = \sum_{i=1}^n a_i u_i \in \mathbb{R}^m$. We then have $u \in \text{Rect}(0_m)$ and $h(u) = v$ because $h(u) = Wu + b = \sum_{i=1}^n a_i W_i u_i + b = \sum_{i=1}^n a_i W_i u_i + W^2 0_{m-n} + b$.

$h(u) = \sum_{i=1}^n a_i W_i V(1_i - \sum_{i=1}^n b_i a_i) = \sum_{i=1}^n a_i 1_i - b + b = v$.

Now let $u = [- (Vb)^T 0_{m-n}^T]^T \geq 0_m$, we then have $h(u) = Wu + b = - W_1 Vb + W^2 0_{m-n} + b = 0_n$.

Therefore, we reach the conclusion.

The matrix $W_1$ whose inverse $V$ is a non-negative matrix as in Corollary 25 is known as a monotone (inverse-positive) matrix (Fujimoto & Ranade, 2004), which forms a supper class of M-matrices (Plemmons, 1977).
Lemma 26. Assume $U \subseteq \text{Rect}(0) \subseteq \mathbb{R}^n$ is a path-connected set. If $u \neq 0$ (exists negative coordinate) and $u \in \hat{\sigma}^{-1}(U)$, the segment $[\hat{\sigma}(u), u] \subset \sigma^{-1}(U)$.

Proof. See the proof in our supplementary material. Given $u \in \mathbb{R}^n$ and $0 \leq \lambda \leq 1$, we verify that $\hat{\sigma}(\lambda u_i + (1 - \lambda) \sigma(u_i)) = \sigma(u_i)$. Let $v = \lambda u_i + (1 - \lambda) \sigma(u_i)$. For $i$ such that $u_i = 0$, let $\hat{\sigma}(u_i) = u_i$, hence $v_i = \lambda u_i + (1 - \lambda) \sigma(u_i) = u_i \hat{\sigma}(v_i)$. For $i$ such that $u_i < 0$ then $\hat{\sigma}(u_i) = 0$, hence $v_i = \lambda u_i + (1 - \lambda) \sigma(u_i) < 0$ and $\hat{\sigma}(v_i) = \hat{\sigma}(v_i) = 0 = \hat{\sigma}(u_i)$. This follows that $\hat{\sigma}(v_i) = \hat{\sigma}(u_i), \forall i$, hence $\sigma(v) = \sigma(u)$ and $v = \lambda u_i + (1 - \lambda) \sigma(u_i) \in \hat{\sigma}^{-1}(U)$. In addition, it is trivial that $U \subseteq \hat{\sigma}^{-1}(U)$ since $U \subseteq \text{Rect}(0) \subseteq \mathbb{R}^n$.

We now prove that if $u \neq 0$ (exists negative coordinate) and $u \in \hat{\sigma}^{-1}(U)$ then the segment $[\hat{\sigma}(u), u] \subset \hat{\sigma}^{-1}(U)$.

Let $v = \lambda u_i + (1 - \lambda) \sigma(u_i) \in [\hat{\sigma}(u), u]$ for some $0 \leq \lambda \leq 1$. Then $\hat{\sigma}(v) = \hat{\sigma}(u) \in U$ which implies $v \in \hat{\sigma}^{-1}(U)$.

Lemma 27. If $U \subseteq \text{Rect}(0) \subseteq \mathbb{R}^n$ is a path-connected set and $C$ is a convex set containing $U$ (i.e., $U \subset C$) then $\hat{\sigma}^{-1}(U) \cap C$ is also a path-connected set provided that $\sigma$ is the ReLU activation function.

Proof. Let $u_1, u_2 \in \hat{\sigma}^{-1}(U) \cap C$. We consider the following cases:

1) $u_1 \geq 0$ and $u_2 \geq 0$:

$\hat{\sigma}(u_1) = u_1 \in U$ and $\hat{\sigma}(u_2) = u_2 \in U$. Since $U$ is path-connected, there exists a path in $U$ connected $\hat{\sigma}(u_1)$ and $\hat{\sigma}(u_2)$ hence this path also connects $u_1$ and $u_2$ in $\hat{\sigma}^{-1}(U) \cap C$ due to $U \subseteq \hat{\sigma}^{-1}(U)$ and $U \subset C$.

2) $u_1 \geq 0$ and $u_2 \neq 0$:

$\hat{\sigma}(u_1) = u_1$ and $\hat{\sigma}(u_2), u_2 \subset \hat{\sigma}^{-1}(U)$ and also $[\hat{\sigma}(u_2), u_2] \subset C$ due to $u_2$, $\hat{\sigma}(u_2), u_2 \in C$ and the convexity of $C$. Since $U$ is path-connected, there exists a path in $U$ connected $\hat{\sigma}(u_1)$ and $\hat{\sigma}(u_2)$ hence this path also connects $u_1$ and $\hat{\sigma}(u_2)$ in $\hat{\sigma}^{-1}(U) \cap C$. Combining this path with the segment $[\hat{\sigma}(u_2), u_2] \subset \hat{\sigma}^{-1}(U) \cap C$, we have a path connecting $u_1, u_2$ in $\hat{\sigma}^{-1}(U) \cap C$.

3) $u_1 \neq 0$ and $u_2 \neq 0$:

$[\hat{\sigma}(u_1), u_1] \subset \hat{\sigma}^{-1}(U) \cap C$ and $[\hat{\sigma}(u_2), u_2] \subset \hat{\sigma}^{-1}(U) \cap C$. The path connecting $\hat{\sigma}(u_1), u_1 \subset \hat{\sigma}^{-1}(U) \cap C$, the path connecting $u_1, u_2$ in $U$, hence in $\hat{\sigma}^{-1}(U) \cap C$ and the segment $[u_2, \hat{\sigma}(u_2)] \subset \hat{\sigma}^{-1}(U) \cap C$.

Theorem 28. Consider a neural network with the ReLU activation function. Let $A_l = h_l(f_{l-1}([\mathbb{R}^d]))$ where $h_l(\cdot) = W_l \times \cdot + b_l$ for every $1 \leq l \leq L$. If $A_l$ is a convex set for every $1 \leq l \leq L$ and satisfies $\hat{\sigma}(A_l) \subset A_l$ for every $1 \leq l \leq L - 1$, the decision region $C_m$ is path-connected for every $1 \leq m \leq M$.

Proof. We first prove that $\hat{\sigma}(A_l) = A_l \cap \text{Rect}(0)$. In fact, we first have $\hat{\sigma}(A_l) \subset A_l \cap \text{Rect}(0)$ (because $\hat{\sigma}$ is ReLU), hence $\hat{\sigma}(A_l) \subset A_l \cap \text{Rect}(0)$. Moreover, let $u \in A_l \cap \text{Rect}(0)$, then $\hat{\sigma}(u) = u$, hence $u \in \hat{\sigma}(A_l)$.

It is obvious that $f_L(C_m) = A_L \cap D_m = U_L$, is a convex set. Let $B_{L-1} = h_{L-1}^1(U_{L-1}) \cap \hat{\sigma}_1(A_{L-1})$, then $h_L$ is an onto affine map from $B_{L-1}$ to $U_L$, hence $B_{L-1}$ is a path-connected subset of $\text{Rect}(0)$. Let $U_{L-1} = \hat{\sigma}_{L-1}^{-1}(B_{L-1} \cap \hat{\sigma}_{L-1}(A_{L-1}))$, then using Lemma 27 with noting that $B_{L-1} \cap \hat{\sigma}_{L-1}(A_{L-1}) \subset A_{L-1}$, we obtain $U_{L-1}$ is path-connected.

Let $B_{L-2} = h_{L-2}^1(U_{L-1}) \cap \hat{\sigma}_2(A_{L-2})$, then we have $B_{L-2}$ is a path-connected subset of $\text{Rect}(0)$. Let $U_{L-2} = \hat{\sigma}_{L-2}(B_{L-2}) \subset A_{L-2}$, then $U_{L-2}$ is a path-connected set. Using the same argument backward the network, we arrive $B_1$ and $U_1$ are path-connected. Finally, from $U_1 = h_1(C_m)$ and $h_1(\cdot)$ is an affine map, we obtain $C_m$ is an open connected set.

Theorem 29. Let the width of the layers of the feedforward neural network satisfy $d = n_0 \geq n_1 \geq n_2 \geq \cdots \geq n_{L-1}$. Let $\sigma_1 : \mathbb{R} \rightarrow \mathbb{R}$ be the ReLU activation function for every layer $1 \leq l \leq L - 1$. If all the weight matrices $(W_l)_{l=1}^{L-1}$ have full rank, $V_l$ is non-negative, and $V_l b_l \leq 0$ where $V_l = (W_l^T)^{-1}$ where $W_l^T$ is defined from $W_l$ as above for every layer $1 \leq l \leq L - 1$ then every decision region $C_m$ (i.e., $1 \leq m \leq M$) is an open connected subset of $\mathbb{R}^d$.

Proof. Let $A_l = h_l(f_{l-1}([\mathbb{R}^d]))$ where $h_l(\cdot) = W_l \times \cdot + b_l$ and $B_l = f_l([\mathbb{R}^d]) = \hat{\sigma}_l(A_l)$ for every $1 \leq l \leq L$. According to Theorem 28, we need to prove $A_l$ is a convex set for every $1 \leq l \leq L$ and $\hat{\sigma}_l(A_l) \subset A_l$ for every $1 \leq l \leq L - 1$.

In fact, we have $A_1 = h_1([\mathbb{R}^d]) = \mathbb{R}^{n_1}$ since $W_1$ has full rank. This follows that $B_1 = \hat{\sigma}_1(A_1) = \text{Rect}(0_{n_1}) \subset A_1$. Corollary 25 gives us the convex set $A_2 = h_2(B_1) = h_2(\text{Rect}(0_{n_1})) \supset \text{Rect}(0_{n_2})$. This follows that $B_2 = \hat{\sigma}_2(A_2) = \text{Rect}(0_{n_2}) \subset A_2$. Using the same argument forward, we arrive $A_{L-1} = h_{L-1}(B_{L-2}) \supset \text{Rect}(0_{n_{L-1}})$. This follows that $B_{L-1} = \hat{\sigma}_{L-1}(A_{L-1}) = \text{Rect}(0_{n_{L-1}}) \subset A_{L-1}$. Finally, $A_L = h_L(B_{L-1})$ is convex. That concludes the proof.

Theorem 30. Let the one hidden layer network satisfy $d = n_0 \geq n_1$ and let $\sigma_1$ be the ReLU activation function and the hidden layer’s weight matrix $W_1$ has full rank. Then every decision region $C_m$ is an open connected subset of $\mathbb{R}^d$ for every $1 \leq m \leq M$.

Proof. The proof of this theorem can be directly derived from Theorem 28 by noting that $A_1 = h_1(f_0([\mathbb{R}^d])) = $
$h_1(\mathbb{R}^d) = \mathbb{R}^{n_1}$ which contains $\hat{\sigma}_1(A_1) = \text{Rect}(0)$.

### 4. Conclusion

Previous work has examined an important theoretical question regarding the capacity of feedforward neural networks to learn connected decision regions. It has been proven that for a particular class of activation functions including leaky ReLU, neural networks having a pyramidal structure (i.e., no layer has more hidden units than the input dimension), produce necessarily connected decision regions. In this paper, we significantly extend this result to a more general theory by providing the sufficient and necessary conditions under which the decision regions of a neural network are connected and then developed main theoretical results for neural networks’ capacity to learn connected regions under a wide range choice for activations functions that were not possible to study before, namely ReLU, sigmoid, tanh, softplus, and exponential linear function.

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