Shallow Neural Network can Perfectly Classify an Object following Separable Probability Distribution

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Motivation

Problem in Machine Learning (ML)
- Choosing an architecture is very burdensome

Research Question
- From given data, can we find a proper architecture?
- What is a sufficient size of it?
Prior Works

- Universal Approximation Theorem
  "2-layer NN can approximate any function.."

  → Just feasibility

- C. Zhang et al., *Understanding deep learning requires rethinking generalization*, ICLR’17
  constructed 2-layer ReLU NN with $2n + d$ weights to fit a dataset with $n$ finite samples in $\mathbb{R}^d$

- H. Valvi and P. J. Ramadge, *An upper-bound on the required size of a neural network classifier*, ICASSP’18
  extended the result considering the separability of a finite dataset

  → Just finite samples

Can we guarantee the generalization beyond a finite dataset?
Our Purpose: Generalization

Can we guarantee the generalization beyond a finite dataset?

- An architecture which fits any datasets from a good distribution

For the rest,

- Simple Separability
- 2-layer NN for Simple Separability
- Extended Separability
- 4-layer NN for Extended Separability
Definition 1

Let $\mathcal{X} \subset \mathbb{R}^d$ and $\mathcal{Y} = [1 : c]$. A distribution $D$ over $\mathcal{X} \times \mathcal{Y}$ is \textit{k-separable with $\delta$-margin} (for some $\delta > 0$) if there exist a projection vector $a \in \mathbb{R}^d$ with $\|a\|_2 = 1$ and constants $b_1 < b_2 < \cdots < b_{k+1}$ such that, for $\mathcal{X}_i := \{x \in \mathcal{X} : b_i + \delta < a^T x < b_{i+1} - \delta\}$, $i \in [1 : k]$,

1. $\mathbb{P}(x,y) \sim D (y = y_i \mid \mathcal{X}_i) = 1$ for some $y_i \in \mathcal{Y}$,
2. $\mathbb{P}(x,y) \sim D \left( \bigcup_{i=1}^{k} \mathcal{X}_i \right) = 1$. 

$\{x \in \mathcal{X} : \mathbb{P}_{(x,y) \sim D} (y = 1) > 0\}$  $\{x \in \mathcal{X} : \mathbb{P}_{(x,y) \sim D} (y = 2) > 0\}$  $\{x \in \mathcal{X} : \mathbb{P}_{(x,y) \sim D} (y = 3) > 0\}$
**Simple Separability**

**Definition 1**

Let $\mathcal{X} \subset \mathbb{R}^d$ and $\mathcal{Y} = [1 : c]$. A distribution $D$ over $\mathcal{X} \times \mathcal{Y}$ is $k$-separable with $\delta$-margin (for some $\delta > 0$) if there exist a projection vector $a \in \mathbb{R}^d$ with $\|a\|_2 = 1$ and constants $b_1 < b_2 < \cdots < b_{k+1}$ such that, for $X_i := \{x \in \mathcal{X} : b_i + \delta < a^T x < b_{i+1} - \delta\}$, $i \in [1 : k]$, 

1. $\mathbb{P}(x,y) \sim D (y = y_i \mid X_i) = 1$ for some $y_i \in \mathcal{Y}$,
2. $\mathbb{P}(x,y) \sim D (\bigcup_{i=1}^k X_i) = 1$.
2-layer NN for Simple Separability

$D$: $k$-separable with $\delta$-margin distribution, $a \in \mathbb{R}^d$: projection vector, $\{b_1, \ldots, b_{k+1}\}$: boundary of intervals

For $(x, y) \in \mathcal{X} \times \mathcal{Y}$, $x$: input, $y$: label, $f(y) \in \mathbb{R}^m$: desired output of NN ($f: \mathcal{Y} \to \mathbb{R}^m$ is injective)

**Theorem 1**

For any $\epsilon > 0$, the 2-layer neural network, $g: \mathcal{X} \to \mathbb{R}^m$ with parameters $a \in \mathbb{R}^d$, $\{b_1, \ldots, b_k\}$,

$$W = \begin{bmatrix} f(y_1)^T \\ f(y_2)^T - f(y_1)^T \\ \vdots \\ f(y_k)^T - f(y_{k-1})^T \end{bmatrix} = [w_1 \ w_2 \ \cdots \ w_m], \text{ and}$$

$$c_s = \frac{1}{\delta} \log \left( \left( \frac{\sqrt{k} \cdot \max_{1 \leq j \leq m} \|w_j\|_2}{\epsilon} \right) \right)$$

satisfies

$$\mathbb{P}_{(x, y) \sim D} \left( \max_{1 \leq j \leq m} |g_j(x) - f_j(y)| > \epsilon \right) = 0$$

where $f_j$ and $g_j$ denote the $j$-th components of $f$ and $g$, respectively.

This network is specified by total $(d + (m + 1)k)$ parameters.
Main Idea: Saturation of Sigmoid through Scaling

Output: \( \rho(a^T x - b_1) \)
Main Idea: Saturation of Sigmoid through Scaling

Output: \( \rho(c_s(a^T x - b_1)) \)

\[
\rho(c_s(a^T x - b_1)) \\
\rho(a^T x - b_1)
\]

\[
0 \leq a^T x - b_1 \times c_s \leq 1
\]
Group Behavior in Hidden Layer as $c_s \to \infty$

We can compute $W$ s.t.

$$
\begin{bmatrix}
-h_1 \\
-h_2 \\
\vdots \\
-h_k \\
\end{bmatrix}
W =
\begin{bmatrix}
-f(y_1)^T \\
-f(y_2)^T \\
\vdots \\
-f(y_k)^T \\
\end{bmatrix}
$$

since the left matrix in LHS is invertible.

$h_1 = [1 0 0 0 0]$ $h_2 = [1 1 0 0 0]$ $h_3 = [1 1 1 0 0]$ $h_4 = [1 1 1 1 0]$ $h_5 = [1 1 1 1 1]$
Allowing $\epsilon$ Errors in Output Layer

$c_s \to \infty$ is impractical $\Rightarrow$ Can we confine $c_s$ by allowing some error?

\[
1 - e^{-t} < \rho(t) = 1/(1 + e^{-t}) < e^t
\]

\[
err < e^{-c_s \delta}
\]

If $c_s \geq (1/\delta) \log \left( \left( \sqrt{k} \cdot (\max_{1 \leq j \leq m} ||w_j||_2) \right) / \epsilon \right)$,

then, in each node of output layer, $err \leq \epsilon / \left( \sqrt{k} \cdot (\max_{1 \leq j \leq m} ||w_j||_2) \right)$

Inference and Information for Data Science Lab
2-layer NN for Simple Separability - Simulation

- $f$: one-hot encoding $\Rightarrow$ maximum allowable error: $\epsilon = 1/2$
- Synthetic data: 6k samples from a 20-separable with 0.1-margin distribution
- Sufficient $c_s = (1/\delta) \log \left( \left( \sqrt{k} \cdot \max_{1 \leq j \leq m} \|w_j\|_2 \right) / \epsilon \right) \approx 11.02$
What if the data does not follow simple separability?

- Different colors for different labels
What if the data does not follow simple separability?

- Different colors for different labels
**Extended Separability**

**Definition 2**

Let $\mathcal{X} \subset \mathbb{R}^d$ and $\mathcal{Y} = [1 : c]$. A distribution $D$ over $\mathcal{X} \times \mathcal{Y}$ is \((k_1, k_2, \cdots, k_n)\)-separable with $\delta$-margin (for some $\delta > 0$) if there exist projection vectors $a_1, a_2, \cdots, a_n \in \mathbb{R}^d$ with $\|a_s\|_2 = 1$ and constants $b_{s,1} < b_{s,2} < \cdots < b_{s,k_s+1}$ for $1 \leq s \leq n$, such that, for $\mathcal{X}_i = \{x \in \mathcal{X} : b_{s,i_s} + \delta < a_s^T x < b_{s,i_s+1} - \delta \text{ for } 1 \leq s \leq n\}$, $\mathbf{i} = (i_1, i_2, \cdots, i_n)$, with $i_s \in [1 : k_s]$ for $1 \leq s \leq n$,

1. $\mathbb{P}_{(x,y) \sim D}(y = y_i \mid \mathcal{X}_i) = 1$ for some $y_i \in \mathcal{Y}$,
2. $\mathbb{P}_{(x,y) \sim D}(\bigcup_i \mathcal{X}_i) = 1$. 
4-layer NN for Extended Separability

\( D: (k_1, k_2, \cdots, k_n) \)-separable with \( \delta \)-margin distribution, \( a_1, a_2, \cdots, a_n \in \mathbb{R}^d \): projection vectors
For \( (x, y) \in \mathcal{X} \times \mathcal{Y} \), \( x \): input, \( y \): label, \( f(y) \in \mathbb{R}^m \): desired output of NN (\( f: \mathcal{Y} \to \mathbb{R}^m \) is injective)

**Theorem 2**

For any \( \epsilon > 0 \), there exists a 4-layer NN, \( g : \mathcal{X} \to \mathbb{R}^m \), with \((n(d+1) + 2 \sum_{s=1}^{n} k_s + (m+1) \prod_{s=1}^{n} k_s)\) parameters such that

\[
P_{(x,y) \sim D} \left( \max_{1 \leq j \leq m} |g_j(x) - f_j(y)| > \epsilon \right) = 0
\]

where \( f_j \) and \( g_j \) denote the \( j \)-th components of \( f \) and \( g \), respectively.
2 Steps to Construct the 4-layer NN

Step 1. Mapping to Simple Separable Data

Step 2. Constructing 2-layer NN for Simple Separability (Thm. 1)
Step 1. Mapping to Simple Separable Data

Lemma

For data \((x, y)\) following a distribution \(D\) that is \((k_1, k_2, \ldots, k_n)\)-separable with \(\delta\)-margin by \(n\) projection vectors \((a_1, \ldots, a_n)\), there exists a 2-layer NN that implements \(p : \mathcal{X} \rightarrow \mathbb{R}^n\) such that \((p(x), y)\) follows a distribution \(D'\) that is \((\prod_{s=1}^{n} k_s)\)-separable with \(\left(\frac{1}{4\sqrt{n}}\right)\)-margin by a projection vector \(a = \frac{1}{\sqrt{n}}[1, 1, \ldots, 1]^T \in \mathbb{R}^n\).

Main Idea

- Projection into \(a = \frac{1}{\sqrt{n}}[1, 1, \ldots, 1]^T\) is a (scaled) component-wise summation
- Each parallel NN (approximately) outputs differently scaled integers ex) \(\{0, 1, \ldots, k_1\}\) for \(a_1\), \(\{0 \times k_1, 1 \times k_1, \ldots, k_2 \times k_1\}\) for \(a_2\), and so on
4-layer NN for Extended Separability

\[ D: (k_1, k_2, \cdots, k_n) \text{-separable with } \delta \text{-margin distribution, } a_1, a_2, \cdots, a_n \in \mathbb{R}^d: \text{ projection vectors} \]

For \((x, y) \in \mathcal{X} \times \mathcal{Y}, x: \text{ input, } y: \text{ label, } f(y) \in \mathbb{R}^m: \text{ desired output of NN (} f: \mathcal{Y} \rightarrow \mathbb{R}^m \text{ is injective}) \]

**Theorem 2**

For any \(\epsilon > 0\), there exists a 4-layer NN, \(g: \mathcal{X} \rightarrow \mathbb{R}^m\), with \((n(d+1) + 2 \sum_{s=1}^{n} k_s + (m+1) \prod_{s=1}^{n} k_s)\) parameters such that

\[
P_{(x,y) \sim D} \left( \max_{1 \leq j \leq m} |g_j(x) - f_j(y)| > \epsilon \right) = 0
\]

where \(f_j\) and \(g_j\) denote the \(j\)-th components of \(f\) and \(g\), respectively.
**Conclusion**

- Construct 4-layer sigmoid-type NN that could generalize to any datasets under the separable condition.
- Demonstrate potential benefit of saturation of sigmoid func. in the generalization beyond finite samples.

**Remaining Questions**

- How to find projection vectors and boundaries for given separable dataset?
- Can we approximate a general dataset as a separable one?
  - Error for approximating a Gaussian mixture.

*Full paper in arXiv:1904.09109*