The estimation of training accuracy for two-layer neural networks on random datasets without training

Shuyue Guan · Murray Loew

Abstract Although the neural network (NN) technique plays an important role in machine learning, understanding the mechanism of NN models and the transparency of deep learning still require more basic research. In this study we propose a novel theory based on space partitioning to estimate the approximate training accuracy for two-layer neural networks on random datasets without training. There appear to be no other studies that have proposed a method to estimate training accuracy without using input data or trained models. Our method estimates the training accuracy for two-layer fully-connected neural networks on two-class random datasets using only three arguments: the dimensionality of inputs ($d$), the number of inputs ($N$), and the number of neurons in the hidden layer ($L$). We have verified our method using real training accuracies in our experiments. The results indicate that the method will work for any dimension, and the proposed theory could extend also to estimate deeper NN models. This study may provide a starting point for a new way for researchers to make progress on the difficult problem of understanding deep learning.

Keywords Training accuracy estimation · Neural networks performance · Transparency of neural networks · Explanation/understanding of deep learning · Fully-connected neural networks · Space partitioning

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1 Introduction

In recent years, the neural network (deep learning) technique has played a more and more important role in applications of machine learning. To comprehensively understand the mechanisms of neural network (NN) models and to explain their output results, however, still require more basic research (Roscher et al., 2020). To understand the mechanisms of NN models, that is, the transparency of deep learning, there are mainly three ways: the training process (Du et al., 2018), generalizability (Liu et al., 2020), and loss or accuracy prediction (Arora et al., 2019).

In this study, we create a novel theory from scratch to approximately estimate the training accuracy for two-layer neural networks on random datasets. Its main idea is based on the regions of linearity represented by NN models (Pascanu et al., 2014), which derives from common insights of the Perceptron. Specifically, the studied subjects are:

– **Classifier model**: the two-layer fully-connected neural networks (FCNN) with \( d - L - 1 \) architecture, in which the length of input vectors \( \in \mathbb{R}^d \) is \( d \), the hidden layer has \( L \) neurons (with ReLU activation), and the output layer has one neuron with the Sigmoid function. This FCNN is for two-class classifications and outputs of the FCNN are values in \([0,1]\).

– **Dataset**: \( N \) random (uniformly distributed) vectors in \( \mathbb{R}^d \) belonging to two classes with labels ‘0’ and ‘1’, and the number of samples for each class is the same.

– **Metrics**: training accuracy.

The paradigm we use to study the FCNN is similar to that of research in physics. First, we find a simplified system to examine; second, we create a theory based on several hypotheses to predict or estimate results of the system. Third, for the most important step, we apply experiments to verify the proposed theory by comparing predicted results with real outcomes of the system. If the predictions are close to the real results, we could accept the theory or update it to make predictions/estimates more accurate. Otherwise, we abandon this theory and seek another one.

To the best of our knowledge, only a few studies have addressed the issue of training accuracy prediction/estimation for NN models. Deng et al. (2017) and Istrate et al. (2019) propose LSTM-based frameworks (Peephole and TAP) to predict a NN model’s performance before training the original model but the frameworks still need training by input data before making predictions. And the accuracy prediction method of Unterthiner et al. (2020) requires weights from the trained NN model. None of them, however, estimates training accuracy without using input data nor trained models. Through our method, to estimate the training accuracy for two-layer FCNN on random datasets (two classes) requires only three arguments: the dimensionality of inputs \( d \), the number of inputs \( N \), and the number of neurons in the hidden layer \( L \).

This paper has two contributions: 1) to introduce a novel theory to understand the mechanisms of NN models and 2) by applying that theory, to
estimate the training accuracy for two-layer FCNN on random datasets. This study may raise other questions and discover the starting point of a new way for future researchers to make progress in the understanding of deep learning. In the next section, we will describe the proposed theory to estimate the results of training accuracy.

2 The hidden layer: space partitioning

In general, the output of the \( k \)-th neuron in the first hidden layer is:

\[
s_k(x) = \sigma(w_k \cdot x + b_k)
\]

Where input \( x \in \mathbb{R}^d \); parameter \( w_k \) is the input weight of the \( k \)-th neuron and its bias is \( b_k \). We define \( \sigma(\cdot) \) as the ReLU activation function, defined as:

\[
\sigma(x) = \max\{0, x\}
\]

The neuron can be considered as a hyperplane: \( w_k \cdot x + b_k = 0 \) that divides the input space \( \mathbb{R}^d \) into two partitions (Pascanu et al., 2014). If the input \( x \) is in one (lower) partition or on the hyperplane, then \( w_k \cdot x + b_k \leq 0 \) and then their output \( s_k(x) = 0 \). If \( x \) is in the other (upper) partition, its output \( s_k(x) > 0 \). Specifically, the distance from \( x \) to the hyperplane is:

\[
d_k(x) = \frac{|w_k \cdot x + b_k|}{\|w_k\|}
\]

If \( w_k \cdot x + b_k > 0 \),

\[
s_k(x) = \sigma(w_k \cdot x + b_k) = |w_k \cdot x + b_k| = d_k(x)\|w_k\|
\]

For a given input data point, \( L \) neurons assign it a unique code: \( \{s_1, s_2, \cdots, s_L\} \); some values in the code could be zero. \( L \) neurons divide the input space into many partitions, input data in the same partition will have codes that are more similar because of having the same zero positions. Conversely, it is obvious that the codes of data in different partitions have different zero positions, and the differences (the Hamming distances) of these codes are greater. It is apparent, therefore, that the case of input data separated into different partitions is favorable for classification.

2.1 Complete separation

We suppose \( L \) neurons divide the input space into \( S \) partitions and hypothesize that:

**Hypothesis 1.** For the best performance of classification, all \( N \) input data have been separated in different partitions (named complete separation).
Under this hypothesis, for complete separation, each partition contains at most one data point after space partitioning. Since the position of data points and hyper-planes can be considered (uniformly distributed) random, the probability of complete separation ($P_c$) is:

$$P_c = \left(\frac{S}{N}\right) = \frac{S!}{(S-N)!S^N}$$

(1)

By the Stirling’s approximation,

$$P_c = \frac{S!}{(S-N)!S^N} \approx \frac{\sqrt{2\pi S \left(\frac{S}{e}\right)^S}}{\sqrt{2\pi (S-N) \left(\frac{S-N}{e}\right)^{S-N} S^N}}$$

$$P_c = \left(\frac{1}{e}\right)^N \left(\frac{S}{S-N}\right)^{S-N+0.5}$$

(2)

Let $S = bN^a$ and for a large $N \to \infty$, by Eq. (2), the limitation of complete separation probability is:

$$\lim_{N \to \infty} P_c = \lim_{N \to \infty} \left(\frac{1}{e}\right)^N \left(\frac{bN^a}{bN^a - N}\right)^{bN^a - N + 0.5}$$

(3)

$S > 0$ requires $b > 0$; and for complete separation, $\forall N: S \geq N$ (Pigeonhole principle) requires $a \geq 1$. By simplifying the limit in Eq. (3), we have:  

$$\lim_{N \to \infty} P_c = \lim_{N \to \infty} e^{-\left(\frac{(a-1)N^{2-a}}{a^{\frac{a}{a}}}ight)} \quad \text{when } a > 1$$

$$\text{lim}_{N \to \infty} P_c = 0 \quad \text{when } a = 1$$

(4)

Eq. (4) shows that for large $N$, the probability of complete separation is nearly zero when $1 \leq a < 2$, and close to one when $a > 2$. Only for $a = 2$ is the probability controlled by the coefficient $b$:

$$\lim_{N \to \infty} P_c = e^{-\left(\frac{1}{b}\right)} \quad \text{when } S = bN^2$$

(5)

Although complete separation holds ($\lim_{N \to \infty} P_c = 1$) for $a > 2$, there is no need to incur the exponential growth of $S$ with $a$ when compared to the linear growth with $b$. And a high probability of complete separation does not require even a large $b$. For example, when $a = 2$ and $b = 10$ the $\lim_{N \to \infty} P_c \approx 0.95$.

Therefore, we let $S = bN^2$ throughout this study.

\footnote{A derivation of this simplification is available in the Appendix.}
2.2 Incomplete separation

To increase the $b$ in Eq. (5) can improve the probability of complete separation. Alternatively, to decrease the training accuracy could improve the probability of an incomplete separation, that is, some partitions have more than one data point after space partitioning. We define the separation ratio $\gamma$ ($0 \leq \gamma \leq 1$) for $N$ input data, which means at least $\gamma N$ data points have been completely separated (at least $\gamma N$ partitions contain only one data point). According to Eq. (1), the probability of such incomplete separation ($P_{inc}$) is:

$$P_{inc} = \frac{\binom{S}{\gamma N} \binom{(S-\gamma N)(1-\gamma)^N}{(1-\gamma)^N N^N}}{S^N} = \frac{S! (S-\gamma N)^{1-\gamma N}}{(S-\gamma N)! S^N}$$

(6)

When $\gamma = 1$, $P_{inc} = P_c$, i.e., it becomes the complete separation, and when $\gamma = 0$, $P_{inc} = 1$. We apply Stirling’s approximation and let $S = b N^2$, $N \rightarrow \infty$, similar to Eq. (5), we have:

$$\lim_{N \rightarrow \infty} P_{inc} = e^{\frac{\gamma (\gamma - 2)}{2b}}$$

(7)

2.3 Expectation of separation ratio

In fact, Eq. (7) shows the probability that at least $\gamma N$ data points (when $N$ is large enough) have been completely separated, which implies:

$$P_{inc} (x \geq \gamma) = e^{\frac{\gamma (\gamma - 2)}{2b}} \Rightarrow P_{inc} (x = \gamma) = dP_{inc} (x < \gamma) = d (1 - P_{inc} (x \geq \gamma)) =$$

$$= \frac{d}{d\gamma} \left( 1 - e^{\frac{\gamma (\gamma - 2)}{2b}} \right) = \frac{1 - \gamma}{b} e^{\frac{\gamma (\gamma - 2)}{2b}} = P_{inc} (\gamma)$$

We notice that the equation $P_{inc} (\gamma)$ does not include the probability of complete separation $P_c$ because $P_{inc} (1) = 0$. Hence, $P_{inc} (1)$ is replaced by $P_c$ and the comprehensive probability for the separation ratio $\gamma$ is:

$$P(\gamma) = \begin{cases} P_c & \gamma = 1 \\ \frac{1}{b} e^{\frac{\gamma (\gamma - 2)}{2b}} & 0 \leq \gamma < 1 \end{cases}$$

(8)

Since Eq. (8) is a function of probability, we could verify it by:

$$\int_0^1 P(\gamma)\,d\gamma = P_c + \int_0^1 \frac{1 - \gamma}{b} e^{\frac{\gamma (\gamma - 2)}{2b}}\,d\gamma = e^{-\left(\frac{1}{b}\right)} + \left(1 - e^{-\left(\frac{1}{b}\right)}\right) = 1$$

We compute the expectation of the separation ratio $\gamma$:

$$E[\gamma] = \int_0^1 \gamma \cdot P(\gamma)\,d\gamma = 1 \cdot P_c + \int_0^1 \gamma \cdot \frac{1 - \gamma}{b} e^{\frac{\gamma (\gamma - 2)}{2b}}\,d\gamma$$
\[ E[\gamma] = \frac{\sqrt{2\pi b}}{2} \text{erfi}\left(\frac{1}{\sqrt{2b}}\right) e^{-\left(\frac{1}{2b}\right)} \]  

(9)

where \text{erfi}(x) is the imaginary error function:

\[ \text{erfi}(x) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{x^{2n+1}}{n!(2n+1)} \]

2.4 Expectation of training accuracy

Based on the hypothesis, a high separation ratio helps to obtain a high training accuracy, but it is not sufficient because the training accuracy also depends on the separating capacity of the second (output) layer. Nevertheless, we firstly ignore this fact and reinforce our Hypothesis 1.

**Hypothesis 2.** The separation ratio directly determines the training accuracy.

Then, we will add empirical corrections to our theory to allow it to match the real situations. We suppose that, in the condition of incomplete separation, all completely separated data points can be predicted correctly, and that the other data points have a 50% chance to be predicted correctly (equivalent to a random guess, since the number of samples for each class is the same). Specifically, if \( \gamma N \) data points have been completely separated, the training accuracy \( \alpha \) (based on our hypothesis) is:

\[ \alpha = \frac{\gamma N + 0.5(1 - \gamma) N}{N} = 1 + \frac{\gamma}{2} \]

To take the expectation on both sides, we have:

\[ E[\alpha] = \frac{1 + E[\gamma]}{2} \]  

(10)

Eq. (10) shows the expectation relationship between the separation ratio and training accuracy. After replacing \( E[\gamma] \) in Eq. (10) with Eq. (9), we obtain the formula to compute the expectation of training accuracy:

\[ E[\alpha] = \frac{1}{2} + \frac{\sqrt{2\pi b}}{4} \text{erfi}\left(\frac{1}{\sqrt{2b}}\right) e^{-\left(\frac{1}{2b}\right)} \]  

(11)

To compute the expectation of training accuracy by Eq. (11), we must calculate the value of \( b \). The expectation of training accuracy is a monotonically increasing function of \( b \) on its domain \((0, \infty)\) and its range is \((0.5, 1)\). Since the coefficient \( b \) is very important to estimate the training accuracy, it is also called the ensemble index for training accuracy. This leads to the following theorem:
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**Theorem 1** The expectation of training accuracy for a $d - L - 1$ architecture FCNN is determined by Eq. (11) with the ensemble index $b$.

We suppose that, in the input space $\mathbb{R}^d$, $L$ hyperplanes (neurons) divide the space into $S$ partitions. By the space partitioning theory (Winder, 1966), the maximum number of partitions is:

\[ S = \sum_{i=0}^{d} \binom{L}{i} \]  

(12)

Since:

\[ \sum_{i=0}^{d} \binom{L}{i} = O \left( \frac{L^d}{d!} \right) \]

We let:

\[ S = \frac{L^d}{d!} \]  

(13)

![Fig. 1 Maximum number of partitions in 2-D](image)

Fig. 1 shows that the partition numbers calculated from Eq. (12) and (13) are very close in 2-D. In high dimensions, Eq. (13) is still a relatively tight upper-bound of Eq. (12). By our agreement in Eq. (5), which $S = bN^2$; we have:

\[ b = \frac{L^d}{d!N^2} \]  

(14)

Now, we have introduced our main theory that could estimate the training accuracy for a $d - L - 1$ structure FCNN and two classes of $N$ random (uniformly distributed) data points by using Eq. (14) and (11). For example, a dataset has two-class 200 random data in $\mathbb{R}^3$ (100 samples for each class) and it is used to train a $3 - 200 - 1$ FCNN. In this case,

\[ b = \frac{200^3}{3!200^2} \approx 33.33 \]

Substituting $b = 33.33$ into Eq. (11) yields $E[\alpha] \approx 0.995$, i.e., the expectation of training accuracy for this case is about 99.5%.
3 Empirical corrections

The empirical correction uses results from real experiments to update/correct the theoretical model we have proposed above. The correction is necessary because our hypothesis ignores the separating capacity of the second (output) layer and that the maximum number of partitions is not guaranteed for all situations; e.g., for a large $L$, the real partition number may be much smaller than $S$ in Eq. (12).

In experiments, we train a $d-L-1$ structure FCNN by two-class $N$ random (uniformly distributed) data points in $[0, 1)^d$ with labels ‘0’ and ‘1’ (and the number of samples for each class is equal). The training process ends when the training accuracy converges (loss change is smaller than $10^{-4}$ in 1000 epochs). For each $\{d, N, L\}$, the training repeats several times from scratch, and the recorded training accuracy is the average.

3.1 Two dimensions

In 2-D, by Eq. (14), we have:

$$b = \frac{1}{2} \left( \frac{L}{N} \right)^2$$

If $\frac{L}{N} = c$, $b$ is not changed by $N$. To test this counter-intuitive inference, we let $L = N = \{100, 200, 500, 800, 1000, 2000, 5000\}$. Since $\frac{L}{N} = 1$, $b$ and $E[\alpha]$ are unchanged. But Table 1 shows the real training accuracies vary with $N$. The predicted training accuracy is close to the real training accuracy only at $N = 200$ and the real training accuracy decreases with the growth of $N$. Hence, our theory must be refined using empirical corrections.

| $d$ | $N$ | $L$ | Real Acc | Est. Acc |
|-----|-----|-----|----------|----------|
| 2   | 100 | 100 | 0.844    | 0.769    |
| 2   | 200 | 200 | 0.741    | 0.769    |
| 2   | 500 | 500 | 0.686    | 0.769    |
| 2   | 800 | 800 | 0.664    | 0.769    |
| 2   | 1000| 1000| 0.645    | 0.769    |
| 2   | 2000| 2000| 0.592    | 0.769    |
| 2   | 5000| 5000| 0.556    | 0.769    |

The correction could be applied on either Eq. (14) or (11). We decide to modify the Eq. (14) because the range of function (11) is $(0.5, 1)$, which is an advantage for training accuracy estimation. In Table 1, the real training accuracy decreases when $N$ increases; this suggests that the exponent of $N$
in Eq. (14) should be larger than that of \( L \). Therefore, according to (14), we consider a more general equation to connect the ensemble index \( b \) with parameters \( d \), \( N \), and \( L \):

\[
b = c_d \frac{L^{x_d}}{N^{y_d}}
\]

(15)

**Observation 1.** The ensemble index \( b \) is computed by Eq. (15) with special parameters \( \{x_d, y_d, c_d\} \). \( x_d, y_d \) are exponents of \( N \) and \( L \), and \( c_d \) is a constant. All the three parameters vary with the dimensionality of inputs \( d \).

In 2-D, to determine the \( x_2, y_2, c_2 \) in Eq. (15), we test 81 \( \{N, L\} \), which are the combinations of: \( L, N \in \{100, 200, 500, 800, 1000, 2000, 5000, 10000, 20000\} \). For each \( \{N[i], L[i]\} \), we could obtain a real training accuracy by experiment. Their corresponding ensemble indexes \( b[i] \) are found using Eq. (11). Finally, we determine the \( x_2, y_2, c_2 \) by fitting the \( \frac{1}{b}, N, L \) to Eq. (15); this yields the expression for the ensemble index for 2-D:

\[
b = 8.4531 \frac{L^{0.0744}}{N^{0.6017}}
\]

(16)

The fitting process uses the Curve Fitting Tool (cftool) in MATLAB. Figure 2 shows the 81 points of \( \{N, L\} \) and the fitted curve. The R-squared value of fitting is about 99.8%. The reason to fit \( \frac{1}{b} \) instead of \( b \) is to avoid \( b = +\infty \) when the real accuracy is 1 (it is reachable). In this case, \( \frac{1}{b} = 0 \). Conversely, \( b = 0 \) when the real accuracy is 0.5, which never appears in our experiments. Using an effective classifier rather than random guess makes the accuracy \( > 0.5 \) (\( b > 0 \)), thus, \( \frac{1}{b} \neq +\infty \).

By using Eq. (16) and (11), we estimate training accuracy on selected values of \( N \) and \( L \) in 2-D. The results are shown in Table 2. The differences
between real and estimated training accuracies are small, except the first (row) one. For higher real-accuracy cases (> 0.86), the difference is larger because \( \frac{1}{b} < 1 \) (\( b > 1 \) when the accuracy > 0.86), while the effect is smaller in cases with \( \frac{1}{b} > 1 \) during the fitting to find Eq. (16).

Table 2  Estimated training accuracy results comparison in 2-D. The columns from left to right are dataset size, number of neurons in hidden layer, the real training accuracy, estimated/predicted training accuracy by Eq. (16) and Theorem 1, and (absolute) differences based on estimations between real and estimated accuracies.

| \( d = 2 \) | \( N \) | \( L \) | Real Acc | Est. Acc | Diff |
|-------------|--------|--------|----------|----------|------|
| 115         | 2483   | 0.910  | 0.846    | 0.064    |
| 154         | 1595   | 0.805  | 0.819    | 0.014    |
| 243         | 519    | 0.782  | 0.767    | 0.015    |
| 508         | 4992   | 0.699  | 0.724    | 0.025    |
| 689         | 2206   | 0.665  | 0.685    | 0.020    |
| 1366        | 4133   | 0.614  | 0.631    | 0.016    |
| 2139        | 2384   | 0.578  | 0.593    | 0.015    |
| 2661        | 890    | 0.566  | 0.573    | 0.007    |
| 1462        | 94     | 0.577  | 0.592    | 0.014    |
| 3681        | 1300   | 0.555  | 0.560    | 0.004    |
| 4416        | 4984   | 0.556  | 0.559    | 0.003    |
| 4498        | 1359   | 0.550  | 0.552    | 0.002    |

3.2 Three and more dimensions

We repeat the same processes for 2-D to determine special parameters \( \{x_d, y_d, c_d\} \) in Observation 1 for data dimensionality from 3 to 10. Results are shown in Table 3. The R-squared values of fitting are high.

Table 3 Parameters \( \{x_d, y_d, c_d\} \) in Eq. (15) (Observation 1) for various dimensionalities of inputs are determined by fitting.

| \( d \) | \( x_d \) | \( y_d \) | \( c_d \) | R-squared |
|--------|----------|----------|----------|-----------|
| 2      | 0.0744   | 0.6017   | 8.4531   | 0.998     |
| 3      | 0.1269   | 0.6352   | 15.5690  | 0.965     |
| 4      | 0.2802   | 0.7811   | 47.3261  | 0.961     |
| 5      | 0.5326   | 0.8515   | 28.4495  | 0.996     |
| 6      | 0.4130   | 0.8686   | 61.0874  | 0.996     |
| 7      | 0.4348   | 0.8239   | 33.4448  | 0.977     |
| 8      | 0.5278   | 0.9228   | 61.3121  | 0.996     |
| 9      | 0.7250   | 1.0310   | 82.5083  | 0.995     |
| 10     | 0.6633   | 1.0160   | 91.4913  | 0.995     |

Such results reaffirm the necessity of correction to our theory because, when compared to Eq. (14), parameters \( \{x_d, y_d, c_d\} \) are not \( \{d, 2, \frac{1}{b}\} \). But
the growth of $\frac{xd}{yd}$ is preserved. From Eq. (14),

$$\frac{xd}{yd} = \frac{d}{2}$$

The $\frac{xd}{yd}$ linearly increases with $d$. The real $d$ v.s. $\frac{xd}{yd}$ (Figure 3) shows the same tendency.

![Fig. 3](image_url)

Fig. 3  Plots of $d$ v.s. $\frac{xd}{yd}$ from Table 3. Blue dot-line is linearly fitted by points to show the growth.

Table 3 indicates that $xd$, $yd$, and $cd$ increase almost linearly with $d$. Thus, we apply linear fitting on $d$-$xd$, $d$-$yd$, and $d$-$cd$ to obtain these fits:

$$\begin{align*}
xd &= 0.0758 \cdot d - 0.0349 \quad (R^2 = 0.858) \\
zd &= 0.0517 \cdot d + 0.5268 \quad (R^2 = 0.902) \\
cd &= 9.4323 \cdot d - 8.8558 \quad (R^2 = 0.804)
\end{align*}$$

Eq. (17) is a supplement to Observation 1, which employs empirical corrections to Eq. (14) for determining the ensemble index $b$ of Theorem 1. To associate the two statements, we can estimate the training accuracy for a two-layer FCNN on two-class random datasets using only three arguments: the dimensionality of inputs ($d$), the number of inputs ($N$), and the number of neurons in the hidden layer ($L$), without actual training.

3.3 Testing

To verify our theorem and observation, we firstly estimate training accuracy on a larger range of dimensions ($d = 2$ to $24$) of three situations:

- $N \gg L : N = 10000$, $L = 1000$
- $N \approx L : N = L = 10000$
- $N \ll L : N = 1000$, $L = 10000$
The results are shown in Figure 4. The maximum differences between real and estimated training accuracies are about 0.130 ($N \gg L$), 0.076 ($N \approx L$), and 0.104 ($N \ll L$). There may have two reasons why the differences are not small in some cases of $N \gg L$: 1) in the fitting process, we do not have enough samples of $N \gg L$ so that the corrections are not perfect, 2) the reason why the differences are greater for higher real accuracies is similar to the 2-D situation discussed above.

In addition, we estimate training accuracy on 40 random cases. For each case, the $N, L \in [100, 20000]$ and $d \in [2, 24]$, but principally $d \in [2, 10]$.
because in high dimensions, almost all cases’ accuracies are close to 100% (see Figure 4). Figure 5 shows the results. Each case is plotted with its real and estimated training accuracy. That the overall R-squared value is about 0.955 indicates good estimation.

4 Discussion

Obviously, the empirical corrections are required because the purely theoretical results (to estimate training accuracy by Eq. (14) and Theorem 1) cannot match the real accuracies in 2-D (Table 1). The corrections are not perfect so far, but the corrected estimation method can reflect some characteristics of the real training accuracies. For example, the training accuracies of the $N \gg L$ cases are smaller than those of $N \ll L$, and for specific $N, L$, the training accuracies of higher dimensionality of inputs are greater than those of lower dimensionality. These characteristics are shown by the estimation curves in Figure 4.

Because of the limited number of fitting and testing samples, the empirically-corrected estimation is not very accurate for some cases. And either the theorem, observation or empirical corrections could be improved in the future. The improvements would be along three directions: 1) using more data for fitting, 2) rethinking the space partitioning problem to change the Observation 1. We could use a different approximation formula from the Eq. (13), or involve the probability of reaching the maximum number of partitions. 3) modifying Theorem 1 by reconsidering the necessity of complete separation.
In fact, in real classification problems, complete separation of all data points is a too strong requirement. Instead, to require only that no different-class samples are assigned to the same partition would be more appropriate. We could also involve the capacity of a separating plane (Duda et al., 2012):

\[
f(N, d) = \begin{cases} 
1 & N \leq d + 1 \\
\frac{2}{N^d} \sum_{i=0}^{d} \binom{N-1}{i} & N > d + 1 
\end{cases}
\]

Where \( f(N, d) \) is the probability of the existence of a hyper-plane separating two-class \( N \) points in \( d \) dimensions. An ideal theory is to precisely estimate the accuracy with no, or very limited, empirical corrections. Such theory would be a purely theoretical model derived from several hypotheses and mathematical derivation.

Our proposed estimation theory could extend to multi-layer neural networks. As discussed at the beginning of the second section, \( L \) neurons in the first hidden layer assign every input a unique code. The first hidden layer transforms \( N \) inputs from \( d \)-D to \( L \)-D. Usually, \( L > d \), and the higher dimensionality makes data separation easier for successive layers. Also, the effective \( N \) decreases when data pass through layers if we consider partition merging. Specifically, if a partition and its neighboring partitions contain the same class data, they could be merged into one because these data are locally classified well. The decrease of actual inputs makes data separation easier for successive layers also.

Alternatively, the study of Pascanu et al. (2014) provides a calculation of the number of space partitions (\( S \) regions) created by \( k \) hidden layers:

\[
S = \left( \prod_{i=1}^{k-1} \frac{n_k}{n_0} \right) \sum_{i=0}^{n_0} \binom{n_k}{i}
\]

Where, \( n_0 \) is the size of input layer and \( n_i \) is the \( i \)-th hidden layer. This reduces to Eq. (12) in the present case (\( k = 1, n_0 = d \) and \( n_1 = L \)). The theory for multi-layer neural networks could begin by using the approaches above.

In addition, the proposed theory could also extend to other distributed data besides uniform distribution and/or other types of neural networks by modifying the ways to calculate separation probabilities, such as in Eq. (1) and (6). This study still has several places that are worth attempting to enhance or extend and raises some questions for future works.

5 Conclusions

Our main contribution is to build a novel theory to estimate the training accuracy for two-layer FCNN used on two-class random datasets without using input data or trained models (training); it uses only three arguments: the dimensionality of inputs \( (d) \), the number of inputs \( (N) \), and the number of
neurons in the hidden layer \((L)\). And there appear to be no other studies that have proposed a method to estimate training accuracy in this way.

Our theory is based on the notion that hidden layers in neural networks perform space partitioning and the hypothesis that the data separation ratio determines the training accuracy. Theorem 1 introduces a mapping function between training accuracy and the ensemble index. The ensemble index has a better characteristic than accuracy for prediction because its domain is \((0, \infty)\). It is good for designing prediction models or fitting experimental data. Observation 1 provides a calculation of the ensemble index based on empirical corrections.

The theory has been verified by real training accuracies in our experiments. And it has the potential to estimate deeper neural network models. This study may raise other questions and suggest a starting point for a new way for researchers to make progress on studying the transparency of deep learning.

Appendix: Simplification from Eq. (3) to Eq. (4)

In the paper, Eq. (3):

\[
\lim_{N \to +\infty} P_c = \lim_{N \to +\infty} \left( \frac{1}{e} \right)^N \left( \frac{bN^a}{bN^a - N} \right)^{bN^a - N + 0.5}
\]

Ignoring the constant 0.5 (small to \(N\)),

\[
\lim_{N \to +\infty} P_c = \lim_{N \to +\infty} \left( \frac{1}{e} \right)^N \left( \frac{bN^a}{bN^a - N} \right)^{bN^a - N}
\]

Using equation \(x = e^{\ln x}\),

\[
\lim_{N \to +\infty} P_c = \lim_{N \to +\infty} e^{\ln \left[ \left( \frac{1}{e} \right)^N \left( \frac{bN^a}{bN^a - N} \right)^{bN^a - N} \right]}
\]

\[
\left[ \frac{-N + (bN^a - N) \ln \left( \frac{bN^a}{bN^a - N} \right)}{e^{\ln x}} \right]_{(A)}
\]

Let \(t = \frac{1}{N} \to +0\),

\[
(A) = -\frac{1}{t} + \left( \frac{b}{t^a} - \frac{1}{t} \right) \ln \left( \frac{\frac{b}{t^a}}{\frac{b}{t^a} - \frac{1}{t}} \right) = \frac{(b - t^{a-1}) \ln \left( \frac{b}{b - t^{a-1}} \right)}{t^a} - t^{a-1}
\]

[i] If \(a = 1\),

\[
(A) = \frac{(b - 1) \ln \left( \frac{b}{b - 1} \right) - 1}{t}
\]
In $R$, it is easy to show that, for $b > 0$,

$$1 < \left( \frac{b}{b-1} \right)^{(b-1)} < e$$

Then, we have

$$0 < (B) < 1$$

Therefore,

$$\lim_{N \to +\infty} P_c = e^{-\infty} = 0 \quad \text{(Eq. (4) in paper, when } a = 1)$$

[ii] For $a > 1$, by applying L’Hôpital’s rule several times:

$$\lim_{t \to +0} (A) = \lim_{t \to +0} \frac{(b - t^a)^{a-1} \ln \left( \frac{b}{b - t^a} \right) - t^{a-1}}{t^a}$$

Using L’Hôpital’s rule,

$$= \lim_{t \to +0} \frac{(1-a) t^{a-2} \ln \left( \frac{b}{b - t^a} \right)}{at^{a-1}} = \lim_{t \to +0} \frac{(1-a) \ln \left( \frac{b}{b - t^a} \right)}{at}$$

$$= \lim_{t \to +0} \frac{(a-1)^2}{at} = \lim_{t \to +0} \frac{(a-1)^2}{a(t - bt^{2-a})}$$

Substitute $N = \frac{1}{t}$,

$$\lim_{N \to +\infty} P_c = \lim_{t \to 0} e^{(A)} = \lim_{N \to +\infty} e^{-\frac{(a-1)N^{2-a}}{N}} \quad \text{(Eq. (4) in paper, when } a > 1)$$

When $1 < a < 2$ (and $a = 1$, shown before in [i]),

$$\lim_{N \to +\infty} P_c = e^{-\frac{1}{a\infty}} = 0$$

When $a > 2,$

$$\lim_{N \to +\infty} P_c = e^{-\frac{1}{a}} = 0$$

For $a = 2$,

$$\lim_{N \to +\infty} P_c = e^{-\left( \frac{1}{2} \right)} \quad \text{(Eq. (5) in paper)}$$
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