A Revision of Neural Tangent Kernel-based Approaches for Neural Networks

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Abstract

Recent theoretical works based on the neural tangent kernel (NTK) have shed light on the optimization and generalization of over-parameterized networks, and partially bridge the gap between their practical success and classical learning theory. Especially, using the NTK-based approach, the following three representative results\cite{1,2} were obtained: (1) A training error bound was derived to show that networks can fit any finite training sample perfectly by reflecting a tighter characterization of training speed depending on the data complexity\cite{1}. (2) A generalization error bound invariant of network size was derived by using a data-dependent complexity measure (CMD). It follows from this CMD bound that networks can generalize arbitrary smooth functions\cite{1}. (3) A simple and analytic kernel function was derived as indeed equivalent to a fully-trained network. This kernel outperforms its corresponding network and the existing gold standard, Random Forests, in few shot learning\cite{2,3}. For all of these results to hold, the network scaling factor $\kappa$ should decrease w.r.t. sample size $n$. In this case of decreasing $\kappa$, however, we prove that the aforementioned results are surprisingly erroneous. It is because the output value of trained network decreases to zero when $\kappa$ decreases w.r.t. $n$. To solve this problem, we tighten key bounds by essentially removing $\kappa$-affected values. Our tighter analysis resolves the scaling problem and enables the validation of the original NTK-based results.

1 Introduction

Though neural networks (NNs) have achieved great success in practice, it remains a well-known mystery that over-parameterized NNs (i.e., networks whose width greatly exceed the number of training samples) generalize well and do not suffer from overfitting even with a simple first order optimization\cite{4,5,6,7}, seemingly contradicting the traditional learning theory. To theoretically explain this fact, extensive research has been conducted recently, and one of the main directions is based on the neural tangent kernel (NTK). Given a NN $f_{\theta}(\cdot)$ with parameter $\theta$ and $n$ training inputs $\{x_i\}_{i=1}^n$, the NTK is defined as a Gram matrix $H \in \mathbb{R}^{n \times n}$ induced by the structure of target prediction function (i.e., a NN) whose $(i,j)$-th entry is given by

$[H]_{i,j} := \left(\frac{\partial f_{\theta}(x_i)}{\partial \theta}, \frac{\partial f_{\theta}(x_j)}{\partial \theta}\right)$.  

The NTK was recently introduced in\cite{8} to control the dynamics of learning NNs. In the over-parameterized regime, the trained parameter of NN is close to its initialization, which also makes the
NTK almost unchanged throughout the training process. This stability of NTK allows the learning dynamics of NN to be easily analyzed throughout the training process, thus making it possible to derive training and generalization error bounds by using existing learning theory.

As a representative study using NTK, [1, 2] showed the following important results for over-parameterized NNs:

(a) (Training error bound) A state-of-the-art training error bound reflecting a tighter characterization of training speed than that of recent studies was proposed in [1]. This bound implies that not only is a network able to represent any finite sample perfectly (as shown in [6]), but the speed at which a network learns training samples varies depending on a complexity measure reflecting how well the data is ordered. Thus, it explains why training a NN with random labels leads to slower training and which characteristics the samples should have for fast learning.

(b) (Generalization error bound) A state-of-the-art generalization error bound, referred to as complexity measure of data (CMD) was proposed in [1]. Unlike previous works with large theory-practice gap (e.g. constraints on the true model [9, 10, 11, 12, 13, 14, 15], conditions on the parameters after training [16, 17, 7, 18, 19, 20, 21, 22, 23, 24, 25], and the existence of a certain ground truth sub-network [26]), CMD has no stringent conditions on certain properties of the trained NN and the true model; it only depends on input $x$ and label $y$ of training data and the initial parameter scale $\kappa$ of NN, hence we can calculate the bound before actually training the network. Furthermore, CMD demonstrates that NNs can learn a broad class of smooth functions. In particular, the smoothness requirement of CMD is weaker than that of [26]. With the less restrictive features mentioned above, CMD is considered as one of the most important achievements in the topic of generalizability of over-parameterized NNs and has been the cornerstone of many follow-up studies in recent years [2, 27, 28, 29, 30, 31, 32].

(c) (Kernel regression predictor equivalent to the trained network) A NTK-based kernel regression predictor (NKRP) being equivalent to a fully trained network was proposed in [2]. NKRP is a function simply consisting of two matrix-vector products depending only on the input-label of training instances and structural characteristics of equivalent NN where this equivalent network is a function with arbitrary multiple matrices and nonlinearities. Due to its simplicity, NKRP can be analyzed much more easily than its equivalent or target network while sharing its characteristics. Beyond its theoretical benefits, NKRP is also known to guide a simple but effective neural architecture search (to check which network structure is good for a specific data) [2, 3, 33, 34] and outperform other kernel-based approaches or even the trained networks for some few-shot learning tasks [3, 33].

The above results (a)–(c) derived in [1, 2] provide upper bounds on the training/generalization error or the gap between NKRP and its target NN that are uniformly available over all network scaling (e.g., initialization) parameter $\kappa$. Here, authors of [1, 2] focus only on the case where

$$\kappa = o(1) \text{ w.r.t. } n$$  \hspace{1cm} (2)

in order to have meaningful bounds that can converge to zero as $n$ increases.

Surprisingly, however, we prove in this paper that, contrary to the theories of [1, 2], the training/generalization errors and equivalence bounds in (a)–(c) do not hold when $\kappa$ decreases w.r.t
The high-level reason for this is as follows. As trained parameter is known to be close to its initial one in the over-parameterized regime \([8, 1, 2, 32, 35, 36, 37, 11, 15, 31, 28]\), the output value of trained NN \(|f_{\theta}(x)|\) is close to that of its initial NN \(|f_{\theta(0)}(x)|\). Meanwhile, the output value of its initial NN decreases to zero as \(n\) increases if the scale \(\kappa\) of initialization decreases w.r.t. \(n\). Thus, it can not guarantee zero training error under the condition (2), as the output value of trained NN decreases to zero but the target label does not.

We further resolve the above issue and revise the analyses of [1, 2] without major modifications of the original statements. Hence, our revision makes it possible for results (a)–(c) to maintain their original meanings and implications without any issue on decreasing \(\kappa\). Our revised analyses provide tighter results on training/generalization error bounds and on the condition for the equivalence between NKRPE and its target NN. With these improvements, we can guarantee the bounds to converge to zero even when \(\kappa\) is a constant w.r.t. \(n\).

The organization of this paper is as follows. In Section 2, we introduce the training and generalization error bounds in [1] and show how the decreasing \(\kappa\) issue occurs in these bounds and how we can revise them. Similarly in Section 3, we consider NKRPE in [2] and show how we can correct the issue. We conclude the paper in Section 4.

**Notation and setup.** Sets \(\{1, 2, \ldots, i\}\) and \(\{i, i+1, \ldots, j\}\) are denoted by \(\{i\}\) and \(\{i : j\}\), respectively. The Frobenius norm is denoted by \(\|\cdot\|\). For a matrix \(H\), \(\lambda_{\min}(H)\) denotes the smallest eigenvalue of \(H\). Training samples are given as \(n\) input-label pairs \(\{(x_i, y_i)\}_{i=1}^n\) generated independently from a data distribution \(D(x, y)\). For simplicity, we assume that \(\|x\| = 1\) for \(x\) sampled from \(D\). We denote \(d\)-dimensional input features and scalar labels in the training set by \(X = (x_1, \ldots, x_n) \in \mathbb{R}^{d \times n}\) and \(y = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n\), respectively.

## 2 NTK-based Analysis for Training and Generalization Error Bounds

We first review the training and test error bounds of [1] in Section 2.1, and disprove and revise them in Sections 2.2 and 2.3, respectively.

### 2.1 Preliminary: training and generalization error bounds of [1]

Consider a two-layer, ReLU-activated, and scalar output neural network \(f_{W,a}(x)\) as in [1]:

\[
f_{W,a}(x) := \frac{1}{\sqrt{m}} \sum_{r=1}^{m} a_r \sigma(w_r^\top x).
\]

Here \(x \in \mathbb{R}^d\) is a given input vector, \(W = (w_1, \ldots, w_m) \in \mathbb{R}^{d \times m}\) is the weight matrix in the first layer, \(a = (a_1, \ldots, a_l)^\top \in \mathbb{R}^{m}\) is the weight matrix in the second layer, and \(\sigma(\cdot)\) is the ReLU activation. The setting indicates there are \(m\) hidden neurons.

Using \(n\) samples \((X, y)\), we train the neural network (3) so that its prediction function \(f_{W,a}(\cdot)\) minimizes the following squared error

\[
L(W) = \frac{1}{2} \sum_{i=1}^{n} (y_i - f_{W,a}(x_i))^2.
\]
by updating the network parameter $W$ via the discrete time optimization of gradient descent (GD) as

$$W(k + 1) := W(k) - \eta \frac{\partial L(W)}{\partial W}|_{W=W(k)}.$$  

We denote by $u(k) = (u_1(k), ..., u_n(k))^\top = (f_{W(k),a}(x_1), ..., f_{W(k),a}(x_n))^\top \in \mathbb{R}^n$ the network output with trained parameter $W(k)$ at the $k$-th step of GD. The parameter $W$ is assumed to be randomly initialized as $w_r \sim \mathcal{N}(0, \kappa^2 I_d)$ using standard deviation $\kappa$ for $r \in \{m\}$ as in [1]. Each element of $a$ is independently initialized as following unif($\{-1, 1\}$).

By setting the network $f_0(x)$ and its parameter $\theta$ of NTK in (1) as $f_{W,a}(x)$ and $W(0)$, respectively, [1] derived a specific NTK (with $m = \infty$) as Gram matrix $H^* \in \mathbb{R}^{n \times n}$ as follows: given $X = [x_1, ..., x_n]$ of $n$ input training samples, $(i,j)$-th entry of $H^*$ is given by

$$[H^*]_{i,j} := \mathbb{E}_{w \sim \mathcal{N}(0, I_d)}[x_i^\top x_j 1\{w^\top x_i \geq 0, w^\top x_j \geq 0\}]$$

where $1\{\}$ is the indicator function. We use $\lambda_0$ to denote $\lambda_{\text{min}}(H^*)$. Then, all NTKs obtained by updated parameters $\{W(k)\}_{k=0}^\infty$ are near to $H^*$ in the over-parameterized regime. Using this fact and extending [32] to hold for arbitrary $\kappa$, [1] provided the following theorem, which guarantees zero training error with a convergence rate depending on $\lambda_0$.

**Theorem 2.1** [Theorem 3.1 in [1]]. Suppose that $\|y\| = O(\sqrt{n})$, $m = \Omega\left(\max\left(\frac{n^6}{\lambda_0^2 \kappa^2 \delta^2}, \frac{n^2}{\lambda_0^4} \log \left(\frac{n}{\delta}\right)\right)\right)$, $\lambda_0 > 0$, and $\eta = O\left(\frac{\lambda_0}{n}\right)$. Then, with probability at least $1 - \delta$ for $\delta \in (0, 1)$ over the random initialization of $(W(0), a)$, it follows that for any $\kappa$ and all $k \geq 0$,

$$\|y - u(k + 1)\|^2 \leq (1 - \frac{\eta\lambda_0}{2}) \|y - u(k)\|^2.$$  

As a corollary of Theorem 2.1, [1] showed a new training error bound reflecting a tighter characterization of training speed such that its convergence rate is mainly affected by the training data belonging to the top eigenspaces of $H^*$. This bound is given as follows.

**Corollary 2.1** [The training error bound, Theorem 4.1 in [1]]. Suppose all conditions in Theorem 2.1 hold. Then, with probability at least $1 - \delta$ for $\delta \in (0, 1)$ over the random initialization of $(W(0), a)$, for all $k \geq 0$,

$$\frac{1}{\sqrt{n}} \|y - u(k)\| = \sqrt{\frac{1}{n} \sum_{i=1}^n (1 - \eta \lambda_i)^{2k}(v_i^\top y)^2} \pm O\left(\frac{\kappa}{\delta} + \frac{n^3}{\sqrt{m} \lambda_0^2 \kappa \delta^2}\right),$$  

where $\{v_i\}_{i=1}^n$ are orthonormal eigenvectors of $H^*$ and $\{\lambda_i\}_{i=1}^n$ are the corresponding eigenvalues.

This new bound, given as the right-hand side in (6), reflects the convergence rate in more details by using all the spectral information of $H^*$ (i.e., $\{\lambda_i\}_{i=1}^n$), but the training error bound in (5) reflects only the least influential part (i.e., $\lambda_0 = \lambda_n$) among these information. This improvement over Theorem 2.1 allows to demonstrate that true labels yield faster learning speeds than random labels [1, 6]. Meanwhile, for this bound in (6) to converge to zero, its second term must also decrease to zero and the corresponding condition is given as follows.

\[\text{This condition comes from Lemma 3.1 in [32].}\]
Remark. For the error term $\kappa/\delta$ in (6) to decrease to 0 w.r.t. $n$, it should hold that $\kappa = o(1)$ w.r.t. $n$.

Using Theorem 2.1, [1] also derived the following generalization error bound, named complexity measure of data (CMD).

**Corollary 2.2** [The generalization error bound, Theorem 5.1 in [1]]. Suppose that all conditions except $\lambda_0 > 0$ in Theorem 2.1 hold and we fix a failure probability $\delta \in (0, 1)$. Suppose also that $m = \Omega(\kappa^{-2} \text{poly}(n, \lambda_0^{-1}, \delta^{-1}))$. Suppose further that $\lambda_0 > 0$ holds with probability at least $1 - \delta/3$ for $n$ i.i.d. training samples $\{(x_i, y_i)\}_{i=1}^n$ from true model distribution $D$. Consider any loss function $\ell : \mathbb{R} \times \mathbb{R} \to [0, 1]$ that is 1-Lipschitz in the first argument. Then, with probability at least $1 - \delta$ over the random initialization of $(W(0), a)$ and the training samples, the neural network $f_{W(k), a}(x)$ trained by GD for $k \geq \Omega(\frac{1}{\eta \lambda_0} \log \frac{n}{\delta})$ iterations has population loss\

\[
L_D(f_{W(k), a}(x)) \leq \sqrt{\frac{2y^\top H^{-1}y}{n}} + O\left(\sqrt{\frac{n\kappa}{\lambda_0 \delta}}\right) + O\left(\frac{\log n \lambda_0^2}{\delta n}\right) \tag{7}
\]

The CMD bound, given in the right-hand side of (7), only depends on the training samples (e.g., $y, H^\top, \lambda_0$) and $\kappa$. This makes it possible to know whether a NN can generalize without actually training the NN, as mentioned above.

Remark. For the error term $(\sqrt{n\kappa})/(\lambda_0\delta)$ in (7) to decrease to 0 w.r.t. $n$, it should hold that $\kappa = o\left(\frac{\lambda_0}{\sqrt{n}}\right)$.

### 2.2 Disproof of NTK-based training and generalization error bounds

From the remarks above, $\kappa$ should follow $o(1)$ and $o(\lambda_0/\sqrt{n})$ for the training and test errors in (6) and (7) to approach zero, respectively. In fact, we have shown in Figure 1 that $\lambda_0$ does not increase with $n$ in standard benchmark datasets thus $o(\lambda_0/\sqrt{n})$ implies $o(1)$. Thus, $\kappa$ should follow $o(1)$ for both training and test errors in (6) and (7) to approach zero. These conditions on $\kappa$ can be allowed only if the original Theorem 2.1 is valid for such $\kappa$, as Theorem 2.1 says.

However, in this section, we show that Theorem 2.1 actually does not hold under these conditions on $\kappa$ (i.e., decreasing $\kappa$). Toward this, we consider the case where $\lambda_0$ satisfies the following mild condition

\[
\lambda_0 = O(n^\gamma) > 0 \text{ for some constant } \gamma \leq 1. \tag{8}
\]

Under condition (8), we claim that an additional condition for $\kappa$ (i.e., non-decreasing $\kappa$) is needed for the statements in Theorem 2.1 to hold.

**Theorem 2.2.** Suppose the condition (8) holds for a constant $\gamma \leq 1$ and $m = \Omega(n^{3-2\gamma})$. Suppose further $\kappa = o(1)$ for $n$. Then, for any $\eta$ satisfying $0 < \lambda_0 \eta < 2$, there exists a finite integer $k$ (and $n$) with probability at least $1 - \delta$ for $\delta \in (0, 1)$ over the random initialization of $(W(0), a)$ such that

\[
\|y - u(k + 1)\|^2 > \left(1 - \frac{\eta \lambda_0}{2}\right) \|y - u(k)\|^2. \tag{9}
\]

\[\text{[1]}\] claimed that (7) holds for a general loss, but in fact they implicitly assumed squared loss and did not consider a general loss in the proof.
We can see that (5) and (9) are contradictory and hence the following corollaries can be easily derived.

**Corollary 2.3.** *Theorem 2.1 does not hold if the condition $\kappa = o(1)$ w.r.t. $n$ and (8) hold.*

**Corollary 2.4.** *Corollary 2.1 fails to guarantee that NNs attain zero training loss if (8) holds.*

**Corollary 2.5.** *Corollary 2.2 fails to guarantee that NNs attain zero generalization error if $\lambda_0 = O(\sqrt{n}) > 0$.*

The question that naturally arises at this point is how easily the condition (8) is satisfied in practice. In addition to the observation that $\lambda_0$ does not increase with $n$ in practice as shown in Figure 1, we also find a simple sufficient condition for (8) provided in the following proposition:

**Proposition 1.** *Suppose that $n$ input samples are not parallel, i.e., $x_i \neq cx_j$ for any $c \in \mathbb{R}$ and different $i, j \in \{1, \ldots, n\}$. Then, $\lambda_0 = O(\sqrt{n}) > 0$ holds.*

Proposition 1 confirms that the condition $\lambda_0 = O(\sqrt{n}) > 0$ for Corollary 2.5 holds (i.e., Corollary 2.2 fails) easily in the practically common case where the training data is not parallel.

### 2.3 Revising NTK-based training and generalization error bounds

By Theorem 2.2, $\kappa$ should not decrease w.r.t. $n$ (i.e., $\kappa = o(1)$) in order for the statements in Theorem 2.1 to hold. Thus, we derive tighter bounds so that we avoid the case of setting decreasing $\kappa$ (i.e., $\kappa = \Theta(1)$). In fact, [32] already showed that this is possible for Theorem 2.1 with $\kappa = \Theta(1)$.

Here, we revise training and generalization bounds in Corollaries 2.1 and 2.2.

**Theorem 2.3** [Revision of Corollary 2.1]. *Suppose all conditions in Theorem 2.1 hold and $\kappa = \Theta(1)$. Then, with probability at least $1 - \delta$ for $\delta \in (0, 1)$ over the random initialization of $(W(0), a)$, it follows that for all $k \geq 0$,

$$
\frac{1}{\sqrt{n}} \|y - u(k)\| = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (1 - \eta \lambda_i)^{2k} \left( v_i^\top (y - u(0)) \right)^2 + O\left( \frac{n^3}{\sqrt{m \lambda_0^2 \delta^2}} \right)},
$$

where $\{v_i\}_{i=1}^{n}$ are orthonormal eigenvectors of $H^*$ and $\{\lambda_i\}_{i=1}^{n}$ are the corresponding eigenvalues.*
Compared to Corollary 2.1, the training error bound in Theorem 2.3 does not have the term $\kappa/\delta$. Accordingly, this tighter bound can converge to zero as the iteration number $k$ increases even in the case for $\kappa = \Theta(1)$. This is formally stated in the following:

**Proposition 2.** Suppose all conditions in Theorem 2.1 hold, $\kappa = \Theta(1)$, and $m = \Omega(\frac{n^{\kappa+\alpha}}{\lambda_0})$ with any $\alpha > 0$. Then, with probability at least $1 - \delta$ for $\delta \in (0, 1)$ over the random initialization of $(W(0), a)$, the right hand side of (10) converges to zero as $k$ and $n$ increase.

We also revise the CMD bound in Corollary 2.2 as follows, under the condition $\kappa = \Theta(1)$.

**Theorem 2.4 [Revision of Corollary 2.2].** Suppose that all conditions except $\lambda_0 > 0$ in Theorem 2.1 hold and we fix a failure probability $\delta \in (0, 1)$. Suppose also that $\lambda_0 > 0$ holds with probability at least $1 - \delta/3$ for $n$ i.i.d. training samples $\{(x_i, y_i)\}_{i=1}^n$ from $D$, and that $\kappa = \Theta(1)$ and $m = \tilde{O}(\text{poly}(n, \lambda_0^{-1}, \delta^{-1}))$. Then, with probability at least $1 - \delta$ over the random initialization of $(W(0), a)$ and the training samples, it follows that for any $k \geq \Omega(\frac{1}{m\lambda_0} \log \frac{n}{\delta})$,

$$\mathbb{E}_{(x,y) \sim D} \frac{1}{2} | y - f_{W(k), a}(x) |^2 = O \left( \sqrt{\frac{2(y - u(0))^\top H^{-1} (y - u(0))}{n}} \right) + O \left( \frac{\log \frac{n}{\lambda_0 \delta}}{n} \right).$$

(11)

Compared to the original CMD bound in (7), the revised version (11) does not have the second term of (7), $(\sqrt{n}\kappa)/(\lambda_0\delta)$, which is the culprit for CMD to blow up. By applying Corollary 6.2 in [1] to our setting, we can also bound the first term in (11) even with the introduction of $u(0)$ exactly as in the original CMD bound:

**Proposition 3.** Suppose $y_i - u_i(0) = g(x_i) := \sum_j \alpha_j (\beta_j^\top x_i)^{p_j}$ for all $i \in \{n\}$, where for each $j$, $p_j \in \{1, 2, 4, 6, \ldots\}$ and $\alpha_j \in \mathbb{R}$ and $\beta_j \in \mathbb{R}^d$ are any constants w.r.t. $n$. Then,

$$\sqrt{\frac{2(y - u(0))^\top H^{-1} (y - u(0))}{n}} \leq 6 \sum_j p_j |\alpha_j| |\beta_j|^{p_j} \leq 2 \frac{\sum_j p_j |\alpha_j| |\beta_j|^{p_j}}{\sqrt{n}} = O \left( \frac{1}{\sqrt{n}} \right).$$

(12)

In that sense, the revised bound directly improves the CMD (in addition to fixing it) by only removing its second term without sacrificing any additional assumption.

### 3 NTK-based Analysis to Guarantee Equivalence between Trained Network and Kernel Regression Predictor

As a parallel story, we consider in this section the equivalence guarantee between the kernel regression predictor (NKRP) and the target network given in [2]. This guarantee suffers from the same issue as the training and test error bounds considered in the previous section.

#### 3.1 Preliminary: equivalence between trained network and NKRP in [2]

We follow the setting in [2] so that a NN is allowed to have a multi-layer, fully-connected, and $\kappa$-scaled neural network $f_\theta^{(l)}(x)$ mapping $\mathbb{R}^d$ to $\mathbb{R}$ as follows:

$$x^{(l)} := \sqrt{\frac{c_{\sigma}}{m}} \sigma(W^{(l)} x^{(l-1)}) \text{ for } 1 \leq l \leq L$$
$$f_\theta^{(L)}(x) := \kappa W^{(L+1)} x^{(L)}.$$

(13)
where $\kappa > 0$ is a multiplier in order to control the magnitude of NN output, $x = x^{(0)} \in \mathbb{R}^d$ is the input, $L$ is the number of layers in the network, $W^{(l)} \in \mathbb{R}^{d_l \times d_{l-1}}$ ($d_0 = d$, $d_i = m$ for $0 < i \leq L$) is the training weight matrix of the $k$-th layer for $1 \leq l \leq L$, $\sigma(\cdot)$ is the ReLU-activation, and $c_\sigma = (\mathbb{E}_{x \sim \mathcal{N}(0,1)}[\sigma(x)^2])^{-1}$ is a scaling factor to normalize the input and features. Note that this network $f_\theta^\kappa(x)$ is the result of expanding the number of layers and converting $\kappa$ from an initialization value to an explicit scaling factor value in the two-layer network in (3). We define $\theta := \{W^{(l)}\}_{l=1}^{L+1}$ as the set of all training weight matrices. We initialize each element in the set $\theta$ of all training weight matrices independently to follow $\mathcal{N}(0, 1)$.

In order to train the network, we follow the setting in [2] that minimizes the squared loss $L(\theta)$ over the training data with respect to the set $\theta$ of all training parameters in the network

$$L(\theta) := \frac{1}{2} \sum_{i=1}^{n} (f_\theta^\kappa(x_i) - y_i)^2$$

by using the continuous time optimization of GD with infinitesimally small learning rate (i.e., $\frac{\partial \theta(t)}{\partial t} = -\nabla L(\theta(t))$). Then, the NN output at the end of training ($t = \infty$) is given by

$$f^\kappa(x) := \lim_{t \to \infty} f_\theta^\kappa(x).$$

By setting the network $f_\theta(x)$ and its parameter $\theta$ of NTK in (1) as $f_\theta^\kappa(x)$ and $\theta(0)$ in (13), [2] obtained a specific NTK (with $m = \infty$) $H^* \in \mathbb{R}^{n \times n}$ as follows. For $X = [x_1, ..., x_n]$ of $n$ input training samples, $(i, j)$-th entry of $H^*$ is defined by $[H^*]_{i,j} = \Psi^{(L)}(x_i, x_j)$ where the function $\Psi^{(L)}(x, x')$ from $\mathbb{R}^d \times \mathbb{R}^d$ to $\mathbb{R}$ for arbitrary vectors $x, x' \in \mathbb{R}^d$ is defined in the following way:

$$\Sigma^{(0)}(x, x') := x^\top x',$$

$$\Lambda^{(l)}(x, x') := \begin{pmatrix} \Sigma^{(l-1)}(x, x) & \Sigma^{(l-1)}(x, x') \\ \Sigma^{(l-1)}(x', x) & \Sigma^{(l-1)}(x', x') \end{pmatrix},$$

$$\Sigma^{(l)}(x, x') := c_\sigma \mathbb{E}_{(u,v) \sim \mathcal{N}(0,\Lambda^{(l-1)}(x,x'))}[\sigma(u)\sigma(v)],$$

$$\dot{\Sigma}^{(l)}(x, x') := c_\sigma \mathbb{E}_{(u,v) \sim \mathcal{N}(0,\Lambda^{(l-1)}(x,x'))}[\dot{\sigma}(u)\dot{\sigma}(v)],$$

$$\Psi^{(L)}(x, x') := \sum_{l=1}^{L+1} \left( \Sigma^{(l-1)}(x, x') \cdot \prod_{l' = l}^{L+1} \dot{\Sigma}^{(l')} \right)$$

for $\dot{\Sigma}^{(L+1)}(x, x') := 1$. Using the fact the NTK obtained by an updated parameter $\theta(t)$ remains near from $H^*$ for all $t > 0$ in the over-parameterized regime, [2] proved that if $\kappa$ is given as sufficiently small, the fully-trained network $f^\kappa(x_{te}) := \lim_{t \to \infty} f_\theta^\kappa(x_{te})$ is equivalent to the following NKRP

$$f^{ntk}(x_{te}) := \ker(x_{te}, X)^\top \left( H^* \right)^{-1} y$$

where $x_{te} \in \mathbb{R}^d$ is any testing point and $\ker(x_{te}, X) \in \mathbb{R}^n$ is a kernel vector whose $i$-th element is equal to $\Psi^{(L)}(x_{te}, x_i)$. This result is formally given in (20), which is derived as a corollary of the following theorem ensuring zero training error.
Theorem 3.1 [Lemma F.9 in [2]]. Let \( w \leq \text{poly}(1/n, \lambda_0, 1/L, 1/\log(m), \epsilon, 1/\log(1/\delta), \kappa) \). Suppose that \( m \geq \text{poly}(1/w) \). Then, with probability at least \( 1 - \delta \) over random initialization, for all \( t \geq 0 \),
\[
\|u^{\kappa}(t) - y\| \leq \exp(-\frac{1}{2} \kappa^2 \lambda_0^2 t) \|u^{\kappa}(0) - y\|. \tag{18}
\]
Corollary 3.1 [Equivalence between fully-connected/trained network and kernel regression predictor, Theorem 3.2 in [2]]. Fix arbitrary \( \epsilon > 0 \). Suppose that \( m \geq \text{poly}(1/\epsilon, 1/\kappa, L, 1/\lambda_0, n, \log(1/\delta)) \) for \( \lambda_0 := \lambda_{\text{min}}(H^*) \) and \( H^* \) is positive definite where \( [H^*]_{i,j} = \Psi^{(l)}(x_i, x_j) \) for \( i, j \in \{n\}^2 \). Suppose further that
\[
1/\kappa = \text{poly}(1/\epsilon, \log(n/\delta)) \text{ holds for some small constants } \epsilon, \delta > 0. \tag{19}
\]
Then, for any \( x_{te} \in \mathbb{R}^d \) with \( \|x_{te}\| = 1 \), with probability at least \( 1 - \delta \) over the random initialization,
\[
|f^{\kappa}(x_{te}) - f^{ntk}(x_{te})| = O(\epsilon). \tag{20}
\]
Corollary 3.1 shows the gap between NKRP and its target trained network is upper bounded by an arbitrarily controllable value \( \epsilon \) and \( \kappa \) can be set any value decreasing w.r.t. \( n \) as a polynomial function of \( \epsilon \) (i.e., \( \kappa = \text{poly}(\epsilon) \)) according to (19).

Remark. In order for Corollary 3.1 to guarantee \( \epsilon \) converges to zero as \( n \) increases (i.e., \( \epsilon = O(n^{\alpha}) \) for some \( \alpha < 0 \)), from the condition (19), \( \kappa \) should decrease w.r.t. \( n \) as a polynomial function with input \( 1/n \) (i.e., \( \kappa = 1/\text{poly}(1/\epsilon) = 1/\text{poly}(n^{-\alpha}) = \text{poly}(n^{\alpha}) = \text{poly}(1/n) \)).

3.2 Disproof of the existing equivalence guarantee between the neural network and kernel regression predictor

As the above remark implies, \( \kappa \) must be polynomially decreasing to 0 w.r.t. \( n \) (i.e., \( \kappa = \text{poly}(1/n) \)) for Corollary 3.1 to guarantee the equivalence between the NKTP and a trained NN. If it is the case, then Corollary 3.1 provides a remarkable result that NN, regarded as hard to analyze, can be viewed as one of the kernel functions with many known theoretical properties due to their structural simplicity. However, unfortunately in this case of \( \kappa = \text{poly}(1/n) \), the same issue of decreasing \( \kappa \) in the previous section also occurs and one cannot guarantee this equivalence as originally intended. Specifically, we provide a counterexample on condition for \( \kappa \) under which Theorem 3.1 does not hold, as follows.

Theorem 3.2. Suppose all conditions in Theorem 3.1 hold. Suppose further \( \kappa = o\left(\frac{\lambda_0}{\sqrt{n}}\right) \). Then, with probability at least \( 1 - \delta \) over random initialization, there exists \( t \geq 0 \) satisfying
\[
\|u^{\kappa}(t) - y\| > \exp(-\frac{1}{2} \kappa^2 \lambda_0^2 t) \|u^{\kappa}(0) - y\|. \tag{21}
\]
As the fact that (18) and (21) are contradictory implies, Theorem 3.2 implies Theorem 3.1 (hence Corollary 3.1) does not hold if \( \kappa = o(\lambda_0/\sqrt{n}) \). In particular, as the condition \( \kappa = o(\lambda_0/\sqrt{n}) \) is implied by the condition \( \kappa = \text{poly}(1/n) \), therefore we can induce that Corollary 3.1 does not hold in this case (i.e., \( \kappa = \text{poly}(1/n) \)) of \( \kappa \) to guarantee the equivalence. It is formally given as follows.

Corollary 3.2. (Corollary 3.1 does not guarantee the equivalence) Suppose that \( \lambda_0 = O(1) \) for \( n \). Then, Corollary 3.1 fails to guarantee \( \epsilon \) in (20) converges to zero as \( n \) increases.

As previously demonstrated and discussed in Figure 1, \( \lambda_0 = O(1) \) in Corollary 3.2 holds (hence Corollary 3.1 fails) easily in practice.
3.3 Revising the equivalence between the neural network and kernel regression predictor

By Theorem 3.2, $\kappa$ should not decrease w.r.t. $n$ in order for the statements in Theorem 3.1 to hold. Accordingly, by setting $\kappa$ to a constant w.r.t. $n$, we revise and improve Corollary 3.1 so that we have a meaningful bound as follows.

**Theorem 3.3** [Revision of Corollary 3.1]. Fix arbitrary $\epsilon > 0$ and $x_{te} \in \mathbb{R}^d$ with $\|x_{te}\| = 1$. Suppose $m \geq \text{poly}(1/\epsilon, 1/\kappa, L, 1/\lambda_0, n, \log(1/\delta))$ and a matrix $E^*$ satisfying $[E^*]_{i,j} = \Psi(L)(x_i, x_j)$ for $i, j \in \{n + 1\}^2$ and $x_{n+1} := x_{te}$ is positive definite. Suppose further that $\kappa = 1$.

Then, with probability at least $1 - \delta$ over the random initialization, we have

$$|f^\kappa(x_{te}) - f^\text{ntk}(x_{te})| = O(\epsilon).$$

(22)

Compared to Corollary 3.1 by [2], our revised Theorem 3.3 makes $\kappa$ be independent on $\epsilon$ (i.e., (19) is improved to (22)). This seemingly simple improvement offers the following notable advantage. The value $\epsilon$ in Theorem 3.3 can be set any variable decreasing with $n$, which was not possible for Corollary 3.1 as shown in Corollary 3.2. Thus, Theorem 3.3 guarantees a trained network is equivalent to the NKRP for sufficiently large $n$ without facing situations described in Theorem 3.2.

Note finally that the revised theory requires $E^*$ to be positive definite while the original theory needs $H^*$ to be positive definite. While the direct relationship between these two conditions might be a good direction of future research, we here provide a simple practical case where both conditions hold. Specifically, [35] (see Proposition F.1) showed that one can obtain $H^*$ is positive definite under certain conditions if $n$ training samples are not parallel (see Proposition 1 for the definition of parallel), which is easily satisfied in practice. By simply exchanging $H^*$ to $E^*$ in this process, we can also guarantee that $E^*$ is positive definite if $n$ training samples and the test point $x_{te}$ are not parallel.

4 Conclusion

Over-parameterization implies that the output of a trained NN has the same order of magnitude as its initial one. Hence, to ensure that the network can fully represent samples, the network’s initialization or (additional) scaling factor should probably not be set to decrease to zero. Accordingly, beyond the representative NTK-based results considered in this paper, we believe that our approach can be applied to general over-parameterized NNs, by checking whether a similar ‘decreasing $\kappa$’ problem has occurred in recent studies, and if so by using our approach to revise the corresponding optimization and generalization results. We also hope that our study will serve as a useful safeguard for future analyses of over-parameterized networks.

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A Proofs of Section 2

A.1 Additional definitions

We recall weight matrix $W(k)$ at the $k$th step of gradient descent as

$$W(k + 1) := W(k) - \eta \frac{\partial L(W)}{\partial W}|_{W=W(k)}. \quad (24)$$

Furthermore, we define $Z(k) := \frac{\partial u(k)}{\partial \text{vec}(W(k))} \in \mathbb{R}^{md \times n}$. Thus, $Z(k)$ is derived as

$$Z(k) = \frac{1}{\sqrt{m}} \begin{pmatrix} \mathbb{I}_{1,1}(k) a_1 x_1 & \ldots & \mathbb{I}_{1,n}(k) a_1 x_n \\ \mathbb{I}_{m,1}(k) a_m x_1 & \ldots & \mathbb{I}_{m,n}(k) a_m x_n \end{pmatrix} \in \mathbb{R}^{md \times n}, \quad (25)$$

where $\mathbb{I}_{p,q}(k) := 1 \{ x_q^\top w_p(k) \geq 0 \}$.

Then, (24) can be expressed as

$$\text{vec}(W(k + 1)) = \text{vec}(W(k)) - \eta Z(k) (u(k) - y). \quad (26)$$

A.2 Proof of Propositions

In this section, we introduce the proofs of Propositions 1, 2, and 3, which are given sequentially as follows.

**Proposition 4** (Proposition 1). Suppose that $x_i \neq a x_j$ for any $a \in \mathbb{R}$ and different $i, j \in \{n\}^2$. Then, $\lambda_0 = O(\sqrt{n}) > 0$ holds.

*Proof of Proposition 4.* As $\|x_i\| = 1$ for all $i \in \{n\}$, there exists a finite constant $c \leq 1$ such that $\|x_i^\top x_j\| \leq c$ for $i, j \in \{n\}$. From the definition of $H^*$, $\|H^*\|_{i,j} \leq c$ for $i, j \in \{n\}^2$. Let $z \in \mathbb{R}^n$ be a vector whose elements belong to $\{-1/\sqrt{n}, 1/\sqrt{n}\}$. Then, $\|H^* z\| \leq c \sqrt{n} = O(\sqrt{n})$ for $i \in \{n\}$ so that

$$\frac{\|H^* z\|}{\|z\|} = \sqrt{\sum_{i=1}^{n} (H^* z)_i^2} = O(\sqrt{n}). \quad (27)$$

Thus, from the definition of $\lambda_0$ and (27), $\lambda_0$ is upper bounded as

$$\lambda_0 = \min_{v \in \mathbb{R}^n \text{ s.t. } \|v\| = 1} \frac{\|H^* v\|}{\|v\|} \leq \frac{\|H^* z\|}{\|z\|} = O(\sqrt{n}). \quad (28)$$

From Theorem 3.1 in [32], it follows that $\lambda_0 > 0$ if $x_i \neq a x_j$ for any $a \in \mathbb{R}$ and different $i, j \in \{n\}^2$. Thus, the proof is completed. \qed

**Proposition 5** (Proposition 2). Suppose all conditions in Theorem 2.1 hold, $\kappa = \Theta(1)$, and $m = \Omega(\frac{n^{\alpha+\eta}}{\lambda_0})$ with any $\alpha > 0$. Then, with probability at least $1 - \delta$ for $\delta \in (0, 1)$ over the random initialization of $(W(0), a)$, the right hand side of (10) converges to zero as $k$ and $n$ increase.
Proof of Proposition 5. Note that the right hand side of (10) is given as
\[
\sqrt{\frac{1}{n} \sum_{i=1}^{n} (1 - \eta \lambda_i)^{2k} \left( v_i^\top (y - u(0)) \right)^2 + O\left( \frac{n^3}{\sqrt{m \lambda_0^2 \delta^2}} \right).}
\] (29)

Note that the first term in (29) is upper bounded as
\[
\sqrt{\frac{1}{n} \sum_{i=1}^{n} (1 - \eta \lambda_i)^{2k} \left( v_i^\top (y - u(0)) \right)^2} \leq \sqrt{\frac{1}{n} (1 - \eta \lambda_0)^{2k} \| y - u(0) \|} \\ \overset{(a)}{=} O\left( (1 - \eta \lambda_0)^{k} \right),
\] (30)

where (a) follows from Lemma A.2. As it follows from the conditions in Theorem 2.1 that \(0 < (1 - \eta \lambda_0) < 1\) holds, by applying this fact to (30), we obtain that the first term of the right hand side in (10) converges to zero as \(k\) increases.

If \(m = \Omega\left( \frac{n^{\frac{d+\alpha}{2}}}{\lambda_0} \right)\), the second term in (29) is given as
\[
O\left( \frac{n^3}{\sqrt{m \lambda_0^2 \delta^2}} \right) = O\left( \frac{n^{-\frac{2}{d}}}{} \right).
\] (31)

That is, the second term of the right hand side in (10) also converges to zero as \(n\) increases, thereby completing the proof by applying (30) and (31) to (29).

\[\square\]

Proposition 6 (Proposition 3, variant of Corollary 6.2 in [1]). Suppose \(y_i - u_i(0) = g(x_i) := \sum_j \alpha_j (\beta_j^\top x_i)^{p_j}\) for all \(i \in \{n\}\), where for each \(j\), \(p_j \in \{1, 2, 4, 6, \ldots\}\) and \(\alpha_j \in \mathbb{R}\) and \(\beta_j \in \mathbb{R}^d\) are any constants w.r.t. \(n\). Then,
\[
\sqrt{\frac{2(y - u(0))^\top H_{\star}^{-1}(y - u(0))}{n}} \leq \frac{6 \sum_j p_j |\alpha_j| \|\beta_j\|^{p_j}}{\sqrt{n}} = O\left( \frac{1}{\sqrt{n}} \right).
\] (32)

Proof of Proposition 6. The proof is completed by replacing \(y_i\) in Corollary 6.2 in [1] with \(y_i - u_i(0)\) for all \(i \in \{n\}\).

\[\square\]

A.3 Proof of Theorem 2.2

In this section, we prove Theorem 2.2. We first show some technical lemmas.

The following lemma provides an upper bound of the magnitude of the initial NN output.

Lemma A.1. Suppose that \(\{x_j\}_{j=1}^{n}\) of \(n\) training input samples is bounded as \(\max_{j \in \{n\}} \|x_j\| \leq 1\). Then, it follows that with probability at least \(1 - \delta\) over the random initialization of \((W(0), a)\),
\[
\|u(0)\|^2 = O\left( \frac{n \kappa^2}{\delta} \right).
\] (33)
Proof of Lemma A.1. It follows that

\[ \mathbb{E}_a[\|u(0)\|^2] = \mathbb{E}_a[\|f_{W(0)}(x_1), \ldots, f_{W(0)}(x_n)\|^2] \]

\[ = \mathbb{E}_a\left[ \sum_{j=1}^{n} |f_{W(0)}(x_j)|^2 \right] \]

\[ = \mathbb{E}_a\left[ \frac{1}{m} \sum_{j=1}^{n} \left| \sum_{r \in \{1:m\}} a_r \sigma(w_r^\top x_j) \right|^2 \right] \]

\[ = \frac{1}{m} \sum_{j=1}^{n} \sum_{r \in \{1:m\}} \left| \sigma(w_r^\top x_j) \right|^2. \] (34)

Furthermore, it follows that

\[ \frac{1}{m} \sum_{j=1}^{n} \sum_{r \in \{1:m\}} \left| \sigma(w_r^\top x_j) \right|^2 \leq \frac{1}{m} \sum_{j=1}^{n} \sum_{r \in \{1:m\}} \left| w_r^\top x_j \right|^2 \]

\[ \leq \frac{a}{m} \sum_{r=1}^{m} v_r^2, \] (35)

where \( v_r \) for \( r \in \{m\} \) is independently sampled from \( \mathcal{N}(0, \kappa^2) \) and (a) follows from the rotational invariance of Gaussian random vector and the fact that \( w_r \) follows \( \mathcal{N}(0, \kappa^2 I_d) \) for \( r \in \{1:m\} \).

By combining (34) and (35) and using the fact that \( \mathbb{E}[\sum_{r=1}^{m} v_r^2] = m \kappa^2 \), we obtain

\[ \mathbb{E}_{W(0),a}[\|u(0)\|^2] = O(n \kappa^2). \]

Therefore, by using Markov’s inequality, \( \|u(0)\|^2 = O(n \kappa^2 / \delta) \) is satisfied with probability at least \( 1 - \delta \).

Then, by using Lemma A.1, we can also obtain an upper bound of gap between the initial NN output and label as Lemma A.2.

Lemma A.2. Suppose that set \{\( x_j \)\}_{j=1}^{n} of \( n \) training input samples is bounded as \( \max_{j \in \{n\}} \|x_j\| \leq 1 \). If \( \|y\| = O(\sqrt{n}) \) is satisfied, it follows that with probability at least \( 1 - \delta \) over the random initialization of \((W(0), a)\),

\[ \|y - u(0)\|^2 = O\left(\frac{\max(\kappa^2, 1) n}{\delta}\right). \]

Proof of Lemma A.2. It follows from Lemma A.1 that with probability at least \( 1 - \delta \),

\[ 2 \max(\|y\|^2, \|u(0)\|^2) = O\left(\max\left(1, \frac{\kappa^2}{\delta}\right) n\right) = O\left(\frac{\max(\kappa^2, 1) n}{\delta}\right). \] (36)

Then, the proof is completed by applying the following inequality to (36).

\[ \|y - u(0)\|^2 \leq \|y\|^2 + \|u(0)\|^2 \leq 2 \max(\|y\|^2, \|u(0)\|^2) \]

\( \square \)
The following lemma (i.e., Lemma A.3) gives an upper bound of the gap between each trained weight vector and its initialization, when the training loss is reduced by the GD optimization. This lemma is the result of extending the condition for \( \kappa \) to arbitrary \( \kappa > 0 \) from \( \kappa = 1 \), which is given in Corollary 4.1 in [32].

**Lemma A.3** [Variant of Corollary 4.1 in [32]]. We are given arbitrary \( \kappa > 0 \). Suppose that set \( \{ x_j \}_{j=1}^n \) of \( n \) training input samples is bounded as \( \max_{j \in \{n\}} \| x_j \| \leq 1 \). If the following condition holds for \( k' \in \{ 0, 1, \ldots, k - 1 \} \),

\[
\| y - u(k') \|^2 \leq \left( 1 - \frac{\eta \lambda_0}{2} \right)^{k'} \| y - u(0) \|^2, \tag{37}
\]

then for every \( r \in \{ m \} \),

\[
\| w_r(k) - w_r(0) \| \leq 4 \sqrt{n} \| y - u(0) \| \sqrt{m \lambda_0} =: R', \tag{38}
\]

where \( w_j(k) \) is the column of \( W(k) = [w_1(k), \ldots, w_m(k)] \) at the \( k \)-th step of GD.

**Proof of Lemma A.3.** Since

\[
\frac{\partial L(W)}{\partial w_r} = \frac{1}{\sqrt{m}} \sum_{q=1}^{n} (u_q - y_q) a_r x_q 1(w_r^\top x_q \geq 0),
\]

we get

\[
\left\| \frac{\partial L(W(k'))}{\partial w_r(k')} \right\| \leq \frac{\sqrt{n}}{\sqrt{m}} \| y - u(k') \|. 
\]

Thus, we have

\[
\| w_r(k) - w_r(0) \| \leq \eta \sum_{k'=0}^{k-1} \left\| \frac{\partial L(W(k'))}{\partial w_r(k')} \right\|
\]

\[
\leq \eta \sum_{k'=0}^{k-1} \frac{\sqrt{n}}{\sqrt{m}} \| y - u(k') \|
\]

\[
\leq (a) \frac{\sqrt{n}}{\sqrt{m}} \sum_{k'=0}^{k-1} \eta \left( 1 - \frac{\eta \lambda_0}{2} \right)^{k'/2} \| y - u(0) \|
\]

\[
\leq \frac{\sqrt{n}}{\sqrt{m}} \sum_{k'=0}^{k-1} \eta \left( 1 - \frac{\eta \lambda_0}{4} \right)^{k'} \| y - u(0) \|
\]

\[
\leq 4 \sqrt{n} \| y - u(0) \| \sqrt{m \lambda_0},
\]

where (a) follows from (37).

As a result of Lemma A.3, from the following lemma (i.e., Lemma A.4), we can obtain an upper bound of the magnitude of trained NN output, when the training loss is reduced by the GD optimization.
Lemma A.4. We are given arbitrary \( \kappa > 0 \). Suppose that set \( \{ x_j \}_{j=1}^n \) of \( n \) training input samples is bounded as \( \max_{j \in \{n\}} \| x_j \| \leq 1 \). If the following condition holds for \( k' \in \{0, 1, \ldots, k - 1\} \),
\[
\| y - u(k') \|^2 \leq (1 - \frac{\eta \lambda_0}{2})^{k'} \| y - u(0) \|^2,
\]
then, with probability at least \( 1 - \delta \) over the random initialization of \( (W(0), a) \),
\[
\| u(k) \|^2 = O\left( \frac{n^3 \max(\kappa, 1)^2}{m \lambda_0^2 \delta^2} + \frac{n \kappa^2}{\delta^2} \right).
\]

Proof of Lemma A.4. Define a set of all weights whose distance from \( W(0) \) is smaller than \( R' \) as
\[
\Gamma(W(0), R') := \{ \tilde{W} = [\tilde{w}_1, \ldots, \tilde{w}_m] \in \mathbb{R}^{m \times d} | \max_{r \in \{m\}} \| \tilde{w}_r - w_r(0) \| \leq R' \}.
\]
Then, for any matrix \( \tilde{W} = [\tilde{w}_1, \ldots, \tilde{w}_m] \in \mathbb{R}^{m \times d} \) belonging to \( \Gamma(W(0), R') \) and any \( j \in \{n\} \), it follows that
\[
\mathbb{E}_a[f_{\tilde{W}}(x_j)]^2 = \mathbb{E}_a \left[ \frac{1}{m} \left( \sum_{r \in \{m\}} a_r \sigma(\tilde{w}_r^\top x_j) \right)^2 \right]
\]
\[
= \mathbb{E}_a \left[ \frac{1}{m} \left( \sum_{r \in \{m\}} \sigma(\tilde{w}_r^\top x_j)^2 + \sum_{r, r' \in \{m\}, r \neq r'} a_r a_{r'} \sigma(\tilde{w}_r^\top x_j) \sigma(\tilde{w}_{r'}^\top x_j) \right) \right]
\]
\[
= \frac{1}{m} \left( \sum_{r \in \{m\}} \sigma(\tilde{w}_r^\top x_j)^2 \right) + \frac{1}{m} \left( \sum_{r, r' \in \{m\}, r \neq r'} \mathbb{E}_a[a_r a_{r'}] \sigma(\tilde{w}_r^\top x_j) \sigma(\tilde{w}_{r'}^\top x_j) \right)
\]
\[
= \frac{1}{m} \left( \sum_{r \in \{m\}} \sigma(\tilde{w}_r^\top x_j)^2 \right),
\]
where \( (a) \) follows from \( \tilde{w}_r \) and \( \tilde{w}_{r'} \) are independent of the random vector \( a \) (i.e., \( \tilde{w}_r \) and \( \tilde{w}_{r'} \) are only depending on \( W(0) \) and \( R' \) as \( \tilde{W} \) is an arbitrary matrix satisfying \( \tilde{W} \in \Gamma(W(0), R') \)). Thus, by using Markov’s inequality, we obtain with probability at least \( 1 - \delta \) over the random initialization of \( a \),
\[
f_{\tilde{W}}(x_j)^2 \leq \frac{1}{\delta m} \sum_{r=1}^m \sigma(\tilde{w}_r^\top x_j)^2.
\]
Define \( \tilde{u}(W) := (f_{\tilde{W}}(x_1), \ldots, f_{\tilde{W}}(x_n))^\top \in \mathbb{R}^n \). Then, applying the union bound over (43) for \( j \in \{n\} \), the following inequalities hold with probability at least \( 1 - \Omega(\delta) \) over the random
Theorem 2.2. Suppose that \( \|y\| = O(\sqrt{n}) \), \( \lambda_0 = O(n^\gamma) \) > 0 with a constant \( \gamma \leq 1 \), and \( m = \Omega(n^{3-2\gamma}) \). Suppose further that \( \kappa = O(n^\alpha) \) holds for some constant \( \alpha < 0 \). Then, with probability at least \( 1 - \delta \) over the random initialization of \( (W(0), a) \), there exists a finite integer \( k \) such that

\[
\|y - u(k + 1)\|^2 > (1 - \frac{\eta \lambda_0}{2}) \|y - u(k)\|^2, \tag{46}
\]

where \( \eta \) is any constant such that \( 0 < \lambda_0 \eta < 2 \).
Proof. If the following condition (47) holds for \( k' \in \{0, 1, \ldots, \tilde{k} - 1 \} \)
\[
\| y - u(k') \|^2 \leq (1 - \frac{\eta \lambda_0}{2})^k' \| y - u(0) \|^2,
\] (47)
then, with probability at least 1 – \( \delta \) over the random initialization of \((W(0), a)\), it follows that
\[
\| u(\tilde{k}) \|^2 \overset{(a)}{=} O\left(\frac{n^3 \max(\kappa, 1)^2}{m \lambda_0^2 \delta^2} + \frac{n \kappa^2}{\delta^2}\right)
\overset{(b)}{=} O\left(1 + \frac{n \kappa^2}{\delta^2}\right)
= O(1 + n^{1+2a})
= o(n),
\] (48)
where (a) follows from Lemma A.4 and (b) follows from and \( m = \Omega(n^{3-2\gamma}) \).

On the other hand, if the following condition (49) holds for all \( k \in \{0, 1, \ldots\} \)
\[
\| y - u(k) \|^2 \leq (1 - \frac{\eta \lambda_0}{2})^k \| y - u(0) \|^2,
\] (49)
there exists an integer \( \tilde{k} \in \{0, 1, \ldots\} \) (e.g., any \( \tilde{k} > (\eta \lambda_0)/(2 - \eta \lambda_0) \)^{-1} \log(\| y - u(0) \|^2/\epsilon), as derived from (64)) such that for arbitrary small constant \( \epsilon \) invariant of \( n \),
\[
\| y - u(\tilde{k}) \|^2 \leq \epsilon.
\] (50)
As \( \epsilon \) is invariant of \( n \), (50) implies that
\[
\| u(\tilde{k}) \|^2 = \Theta(\| y \|^2).
\] (51)
In the case where \( \tilde{k} = \tilde{k} \) and \( \| y \|^2 = \Theta(n) \), as (50) implies \( \| u(\tilde{k}) \|^2 = \Theta(\| y \|^2) \) in (51) and (47) also implies \( \| u(\tilde{k}) \|^2 = o(n) \) in (48), (50) and (47) are not satisfied at the same time. This is because \( \| u(\tilde{k}) \|^2 = \Theta(\| y \|^2) \) in (51) is not equal to \( \| u(\tilde{k}) \|^2 = o(n) \) in (48) in this case (\( \tilde{k} = \tilde{k} \) and \( \| y \|^2 = \Theta(n) \)).

Then, for any \( \eta \) satisfying that \( 0 < \lambda_0 \eta < 2 \), if (47) with this constant \( \eta \) is satisfied for all \( k' \geq 0 \), there should exist a integer \( \tilde{k} \) satisfying (50), which means that (47) and (50) are satisfied at the same time. Therefore, (47) is not satisfied for some constant \( k' \in \{0, 1, 2, \ldots\} \) and for any \( \eta \) satisfying that \( 0 < \lambda_0 \eta < 2 \).

A.4 Modification of Theorem 4.1 in [32]

In order to prove Theorem 2.4 stated in Section 2.3, we first prove Theorem A.2 in this section, since Theorem 2.4 is proved by using the result of Theorem A.2. Theorem A.2 is the result of extending the condition for \( \kappa \) to \( \kappa = \Theta(1) \) from \( \kappa = 1 \), which is given in Theorem 4.1 in [32]. Therefore, most of the proof processes for Theorem A.2 (and its technical lemmas) are already proved in [32]; we provide them in this section for completeness.

To prove Theorem A.2, we first introduce some technical lemmas.

We introduce the following lemma (i.e. Lemma A.5), which is Lemma 3.1 in [32]. This result provides that the Gram matrix \( H(0) \) obtained in the finite NN width regime is lower bounded as \( \lambda_0 \) and remains near from that in the infinite NN width regime.
Lemma A.5 [Lemma 3.1 in [32]]. Define matrix $H(k) \in \mathbb{R}^{n \times n}$ such that $p, q$-th entry of $H(k)$ is given by

$$H_{pq}(k) := \frac{1}{m} x_p^\top x_q \sum_{r=1}^m [\mathbb{1}\{w_r(k)^\top x_p \geq 0, w_r(k)^\top x_q \geq 0\}], \quad (52)$$

where $w_j(k)$ is the $j$th column vector of $W(k)$ such that $[w_1(k), ..., w_m(k)] = W(k)$. If $m = \Omega(\frac{n^2}{\lambda_0} \log \frac{n}{\delta})$, it follows that with probability at least $1 - \delta$ over the random initialization of $(W(0), a)$, $\|H(0) - H^*\|_2 \leq \frac{\lambda_0}{\sqrt{\kappa}}$ and $\lambda_{\text{min}}(H(0)) \geq \frac{3}{4} \lambda_0$, where $\lambda_{\text{min}}(H(0))$ is the smallest eigenvalue of $H(0)$.

The following lemma (i.e. Lemma A.6) is a direct extension of Lemma 3.2 in [32] with respect to $\kappa$; we further specify $\kappa$ in Lemma A.6 as [32] assume that $\kappa = 1$. This result provides that the induced Gram matrix $H$ is lower bounded by $\lambda_0$ and remains near from the Gram matrix $H(0)$.

Lemma A.6 [Variant of Lemma 3.2 in [32]]. Suppose that $w_1, ..., w_m$ are independently generated from $\mathcal{N}(0, \kappa^2 I)$ and $m = \Omega(\frac{n^2}{\lambda_0^2} \log \frac{n}{\delta})$. Then, with probability at least $1 - \delta$, the following holds. For any set of weight vectors $w_1, ..., w_m \in \mathbb{R}^d$ that satisfies $\|w_r(0) - w_r\| \leq \frac{c \delta \lambda_0}{n} := R$ for any $r \in \{m\}$, some positive constant $c$, then the matrix $H \in \mathbb{R}^{n \times n}$ whose $p, q$-th entry is defined by

$$H_{pq} := \frac{1}{m} x_p^\top x_q \sum_{r=1}^m [\mathbb{1}\{w_r^\top x_p \geq 0, w_r^\top x_q \geq 0\}] \quad (53)$$

satisfies $\|H - H(0)\|_2 \leq \frac{\lambda_0}{\sqrt{\kappa}}$ and $\lambda_{\text{min}}(H) > \frac{\lambda_0}{2}$, where $H(0)$ is defined in (52) and $\lambda_{\text{min}}(H)$ is the smallest eigenvalue of $H$.

Proof of Lemma A.6. The following event is defined as

$$\mathcal{E}_{qr} := \{\exists w : \|w - w_r(0)\| \leq R, \mathbb{1}\{x_q^\top w_r(0) \geq 0\} \neq \mathbb{1}\{x_q^\top w \geq 0\}\}. \quad (54)$$

This event happens if and only if $\|w_r(0)^\top x_q\| \leq R$. Note that $w_r(0)$ follows $\mathcal{N}(0, \kappa^2 I)$. For $q \in \{n\}$, we get

$$P(\mathcal{E}_{qr}) = P_{h \sim \mathcal{N}(0, 1)}(|h| \leq R) \leq \frac{2R}{\sqrt{2\pi \kappa}}. \quad (55)$$

Then, for any $(p, q) \in \{n\}^2$, it follows that

$$\mathbb{E}[|H_{pq}(0) - H_{pq}|] = \mathbb{E}\left[\frac{1}{m} x_p^\top x_q \sum_{r=1}^m [\mathbb{1}\{w_r(0)^\top x_p \geq 0, w_r(0)^\top x_q \geq 0\} - \mathbb{1}\{w_r^\top x_p \geq 0, w_r^\top x_q \geq 0\}]\right]$$

$$\leq \frac{1}{m} \sum_{r=1}^m \mathbb{E}[\mathbb{1}\{\mathcal{E}_{qr} \cup \mathcal{E}_{rqr}\}] \leq \frac{4R}{\sqrt{2\pi \kappa}}. \quad (56)$$

By summing (56) over $(p, q)$,

$$\mathbb{E}\left[\sum_{pq} |H_{pq}(0) - H_{pq}|\right] \leq \frac{4n^2 R}{\sqrt{2\pi \kappa}}.$$
By Markov’s inequality, with probability at least $1 - \delta$ over the random initialization of $(W(0), a)$,

$$\sum_{pq} |H_{pq}(0) - H_{pq}| \leq \frac{4n^2R}{\sqrt{2\pi \kappa \delta}}.$$ 

Then,

$$\|H - H(0)\|_2 \leq \sum_{pq} |H_{pq}(0) - H_{pq}| \leq \frac{4n^2R}{\sqrt{2\pi \kappa \delta}}. \quad (57)$$

Finally, we can obtain a lower bound of the smallest eigenvalue of $H$ ($\lambda_{\min}(H)$) by plugging in $R$ and using Lemma A.5 as follows.

$$\lambda_{\min}(H) \geq \lambda_{\min}(H(0)) - \|H - H(0)\|_2 \geq \lambda_{\min}(H(0)) - \frac{4n^2R}{\sqrt{2\pi \kappa \delta}} \geq \frac{\lambda_0}{2} \quad (58)$$

The following lemma (i.e. Lemma A.7) is a direct extension of Lemma 4.1 in [32] with respect to $\kappa$; we further specify $\kappa$ in Lemma A.7 as [32] assume $\kappa = 1$. We include the proof of Lemma A.7 for completeness.

**Lemma A.7** [Variant of Lemma 4.1 in [32]]. Let $S_q := \{r \in \{m\} : 1 \{E_{qr}\} = 0\}$ and $(S_q)^\perp := \{m\} \setminus S_q$, where $E_{qr}$ is defined in (54). Then, with probability at least $1 - \delta$ over the random initialization of $(W(0), a)$, we have

$$\sum_{q=1}^{n} |(S_q)^\perp| \leq \frac{CmnR}{\delta \kappa} \quad \text{for some positive constant } C > 0.$$ 

**Proof of Lemma A.7.** Note that

$$\mathbb{E}[|(S_q)^\perp|] = \sum_{r=1}^{m} P(E_{qr}) \leq \frac{2mR}{\sqrt{2\pi \kappa}}, \quad (59)$$

where the inequality follows from (55). Then,

$$\mathbb{E}\left[\sum_{q} |(S_q)^\perp|\right] \leq \frac{2mnR}{\sqrt{2\pi \kappa}}, \quad (60)$$

and by Markov’s inequality, with probability at least $1 - \delta$,

$$\sum_{q} |(S_q)^\perp| \leq \frac{CmnR}{\delta \kappa}. \quad (61)$$

By using Lemmas A.5, A.6, and A.7, we prove the following theorem (i.e. Theorem A.2). Note that Theorem A.2 is a direct extension of Theorem 4.1 in [32] with respect to $\kappa$ (from $\kappa = 1$ to $\kappa = \Theta(1)$). In the proof of Theorem A.2, we also add that there exists no contradiction in Theorem 4.1 in [32].
Theorem A.2. \textit{(Modification of Theorem 4.1 in [32])} Suppose that \( \kappa = \Theta(1) \) for \( n \), \( \|y\| = O(\sqrt{n}) \), \( m = \Omega\left(\max\left(\frac{n^6\kappa^2}{\kappa^2+1}, \frac{n^2}{\kappa^2} \log(n) \right)\right) \), set \( \{x_j\}_{j=1}^{n} \) of \( n \) training input samples is bounded as \( \max_{j \in \{n\}} \|x_j\| \leq 1 \), \( \eta = O\left(\frac{\lambda_0}{n^2}\right) \), and \( \lambda_0 = O(n^\gamma) > 0 \) with a constant \( \gamma \leq 1 \). The DNN parameter \( W(k) \) is optimized via the gradient descent with the step size \( \eta = O\left(\frac{\lambda_0}{n^2}\right) \). Then, with probability at least \( 1 - \delta \) over the random initialization of \( (W(0), a) \), it follows that for \( k \in \{0, 1, 2, \ldots\} \),

\[
\|y - u(k)\|_2^2 \leq (1 - \frac{\eta \lambda_0}{2})^k \|y - u(0)\|_2^2 .
\]  

(62)

Proof of Theorem A.2. Using Theorem A.1 and the fact that the set of all conditions of Theorem A.2 implies that of Theorem A.1, we can obtain the fact that \( \kappa \) should not be \( o(1) \) for \( n \), in order to prove that (62) holds for all \( k \geq 0 \). Therefore, we assume that \( \kappa = \Theta(1) \) and prove that (62) holds for all \( k \geq 0 \) in this case.

We first prove that there exists no contradiction when \( \kappa = \Theta(1) \) by assuming that (62) holds for all \( k \geq 0 \). Suppose that \( \hat{k} \) is any integer satisfying

\[
\hat{k} \log(1 - \frac{\eta \lambda_0}{2}) \leq \log\left(\frac{\epsilon}{\|y - u(0)\|^2}\right) ,
\]

(63)

where \( \epsilon \) is arbitrary small constant invariant of \( n \). As \(-\eta \lambda_0 (2 - \eta \lambda_0)^{-1} \leq \log(1 - \frac{\eta \lambda_0}{2})\), the following condition implies (63).

\[
\hat{k} > \left(\frac{\eta \lambda_0}{2}\right)^{-1} \log\left(\frac{\|y - u(0)\|^2}{\epsilon}\right)
\]

(64)

From \( \eta = O\left(\frac{\lambda_0}{n^2}\right) \), (64) is implied by

\[
\hat{k} = \Omega\left(\frac{n^2}{\lambda_0^2} \log\left(\frac{\|y - u(0)\|^2}{\epsilon}\right)\right).
\]

(65)

Then, as we assume that (62) holds for all \( k \geq 0 \), it follows that for any \( \hat{k} \) satisfying (65),

\[
\|y - u(\hat{k})\|_2^2 \leq \epsilon.
\]

(66)

This implies that the value of \( \|y - u(\hat{k})\|_2^2 \) can be arbitrarily reduced if integer \( \hat{k} \) is sufficiently large. As \( \epsilon \) is arbitrary small and invariant of \( n \), there exists a pair of \( (\epsilon, \hat{k}) \) such that the following conditions hold at the same time:

\[
\|y - u(\hat{k})\|_2^2 \leq \epsilon \text{ and } \|u(\hat{k})\|_2^2 = \Theta(\|y\|_2^2).
\]

(67)

On the other hand, it follows from Lemma A.4 that for \( \hat{k} \) satisfying (67), with probability at least \( 1 - \delta \) over the random initialization of \( (W(0), a) \), the integer \( \hat{k} \) satisfying (67) should also satisfy

\[
\|u(\hat{k})\|_2^2 = O\left(\frac{n^3 \max(\kappa, 1)^2}{m \lambda_0^2 \delta^2} + \frac{n \kappa^2}{\delta^2}\right) \overset{(a)}{=} O(\kappa^2 n),
\]

(68)

where (a) follows from \( m = \Omega\left(\frac{n^6}{\lambda_0^3 \beta}\right) \).
Since we assume $\kappa = \Theta(1)$ for $n$, there exists no contradiction such that \((67)\) is contrary to \((68)\), whereas it can happen when we assume that $\kappa = o(1)$ for $n$ and $\|y\|^2 = \Theta(n)$ (Theorem A.1).

Now we prove that \((62)\) holds for all $k \geq 0$. This proof is based on that of Theorem 4.1 in [32]. To do this, we use the induction hypothesis. We assume that $k = 0$. Then, \((69)\) holds for $k' \in \{0, 1, ..., k\} = \{0\}$.

\[
\|y - u(k')\|^2 \leq (1 - \frac{\eta \lambda_0}{2})^k' \|y - u(0)\|^2 \tag{69}
\]

Next, we assume that $k$ is an integer satisfying $k > 0$. We assume that for $k' \in \{0, 1, ..., k\}$, it holds

\[
\|y - u(k')\|^2 \leq (1 - \frac{\eta \lambda_0}{2})^{k'} \|y - u(0)\|^2 . \tag{70}
\]

The gradient descent of training loss $L(W)$ with respect to the parameter $w_r$ for $r \in \{m\}$ can be derived as

\[
\frac{\partial L(W)}{\partial w_r} = \frac{1}{\sqrt{m}} \sum_{q=1}^{n} (u_q - y_q)a_r x_q 1\{w_r^\top x_q \geq 0\} . \tag{71}
\]

We define the event

\[
E_{qr} := \{\exists w : \|w - w_r(0)\| \leq R, 1\{x_q^\top w_r(0) \geq 0\} \neq 1\{x_q^\top w \geq 0\}\}.
\]

And we define $S_q := \{r \in \{m\} : 1\{E_{qr}\} = 0\}$, $(S_q)^\perp := \{m\} \setminus S_q$, and $R := \frac{c_0 \lambda_0 \log n}{n^2}$ for some positive constant $c$. Then,

\[
u_q(k + 1) - u_q(k) = \frac{1}{\sqrt{m}} \sum_{r=1}^{m} a_r \left( \sigma(w_r(k) + 1) x_q - \sigma(w_r(k) x_q) \right)
\]

\[
= \frac{1}{\sqrt{m}} \sum_{r=1}^{m} a_r \left( \sigma \left( (w_r(k) - \eta \frac{\partial L(W(k))}{\partial w_r(k)})^\top x_q \right) - \sigma(w_r(k) x_q) \right)
\]

\[
= I_1^q + I_2^q ,
\]

where

\[
I_1^q := \frac{1}{\sqrt{m}} \sum_{r \in S_q} a_r \left( \sigma \left( (w_r(k) - \eta \frac{\partial L(W(k))}{\partial w_r(k)})^\top x_q \right) - \sigma(w_r(k) x_q) \right)
\]

\[
I_2^q := \frac{1}{\sqrt{m}} \sum_{r \in (S_q)^\perp} a_r \left( \sigma \left( (w_r(k) - \eta \frac{\partial L(W(k))}{\partial w_r(k)})^\top x_q \right) - \sigma(w_r(k) x_q) \right).
\]

Then, it follows that for some positive constant $C$, with probability at least $1 - \delta$ over the
random initialization of \((W(0), a)\),

\[
|I_2^q| \leq \frac{\eta}{m} \sum_{r \in (S_q)^\perp} |\frac{\partial L(W(k))}{\partial w_r(k)} x_q |
\]

\[
\leq \frac{\eta \| (S_q)^\perp \|}{\sqrt{m}} \max_{r \in \{m\}} \| \frac{\partial L(W(k))}{\partial w_r(k)} \|
\]

\[
\leq \frac{\eta \sqrt{m} \| (S_q)^\perp \| \| y - u(k) \|}{m}
\]

(a) \[
\leq \frac{C \eta m^{3/2} R \| y - u(k) \|}{\delta \kappa},
\]

(b) \[
(72)
\]

where (a) follows from (71) and (b) follows from Lemma A.7.

To analyze \(I_1^q\), by Lemma A.3 and the assumption (70), we obtain that \(\| w_r(k + 1) - w_r(0) \| \leq R'\) and \(\| w_r(k) - w_r(0) \| \leq R'\) for all \(r \in S_q\). Note that \(R' < R\), which is equivalent to

\[
R' := \frac{4 \sqrt{m} \| y - u(0) \|}{\delta \kappa} 
\]

\[
< R := \frac{c k \delta \lambda_0}{n^2} 
\]

\[
\Rightarrow m = \Omega \left( \frac{n^5 \| y - u(0) \|^2}{\lambda_0^4 \kappa^2 \delta^2} \right).
\]

Note that from Lemma A.2 and the assumption \(\kappa = \Theta(1), \| y - u(0) \|^2 = O(\kappa^2 n/\delta)\) with probability at least \(1 - \delta\) over the random initialization of \((W(0), a)\). Thus, it follows that

\[
m = \Omega \left( \frac{n^5 \| y - u(0) \|^2}{\lambda_0^4 \kappa^2 \delta^2} \right) = \Omega \left( \frac{n^6}{\lambda_0^4 \delta^2} \right).
\]

(73)

Since \(R' < R\), for \(r \in S_q\),

\[
1 \{ w_r(k + 1)^\top x_q \geq 0 \} = 1 \{ w_r(k)^\top x_q \geq 0 \}.
\]

Thus,

\[
I_1^q = \frac{\eta}{m} \sum_{p=1}^{n} x_q^\top x_p (u_p(k) - y_p(k)) \sum_{r \in S_q} 1 \{ w_r(k + 1)^\top x_q \geq 0, w_r(k + 1)^\top x_p \geq 0 \}
\]

\[
= -\eta \sum_{p=1}^{n} (u_p(k) - y_p(k)) (H_{qp}(k) - H_{qp}^\perp(k)),
\]

where

\[
H_{ij}(k) := \frac{1}{m} x_i^\top x_j m \sum_{r=1}^{m} [1 \{ w_r(k)^\top x_i \geq 0, w_r(k)^\top x_j \geq 0 \}]
\]

\[
H_{ij}^\perp(k) := \frac{1}{m} x_i^\top x_j \sum_{r \in (S_q)^\perp} [1 \{ w_r(k)^\top x_i \geq 0, w_r(k)^\top x_j \geq 0 \}].
\]

(74)

By using Lemma A.7, it follows that with probability at least \(1 - \delta\) over the random initialization of \((W(0), a)\),

\[
\| H^\perp(k) \|_2 \leq \sum_{(q,p) = (1,1)}^{(n,n)} \| H_{qp}^\perp(k) \| \leq \frac{n \sum_{q=1}^{n} |(S_q)^\perp|}{m} \leq \frac{C n^2 R}{\delta \kappa}.
\]

(75)
By using (71), we get
\[ \|u(k+1) - u(k)\|_2^2 \leq \eta^2 \sum_{q=1}^{n} \left( \sum_{r=1}^{m} \left\| \frac{\partial L(W(k))}{\partial w_r(k)} \right\|_2^2 \right)^2 \leq \eta^2 n^2 \|y - u(k)\|^2. \] (76)

Note that \( m = \Omega\left(\frac{n^6}{\lambda_0^2}\right) \) in (73) implies the condition \( m = \Omega\left(\frac{n^2}{\lambda_0^2} \log\left(\frac{n}{\lambda_0}\right)\right) \) in Lemma A.6 (by using \( \lambda_0 = O(n^7) > 0 \) with a constant \( \gamma \leq 1 \)). Thus, we can use Lemma A.6. From Lemma A.6 and the fact that \( R' < R \), we get
\[ \lambda_{\min}(H(k)) > \frac{\lambda_0}{2}, \] (77)
where \( \lambda_{\min}(H(k)) \) is the smallest eigenvalue of \( H(k) \). Then, by using union bound, the following inequalities hold with probability at least \( 1 - \Omega(\delta) \) over the random initialization of \((W(0), a)\).
\[
\|y - u(k+1)\|_2^2 = \|y - u(k)\|_2^2 - 2(y - u(k))^T(u(k+1) - u(k)) + \|u(k+1) - u(k)\|_2^2
\]
\[= \|y - u(k)\|_2^2 - 2\eta(y - u(k))^T H(k)(y - u(k))
\]
\[+ 2\eta(y - u(k))^T H^{-1}(k)(y - u(k)) - 2(y - u(k))^T I_2 + \|u(k+1) - u(k)\|_2^2
\]
\[\leq (1 - \eta\lambda_0 + \frac{2C\eta m^2 R}{\delta\kappa} + \frac{2C\eta m^{3/2} R}{\delta\kappa} + \eta^2 n^2) \|y - u(k)\|_2^2 \]
\[\leq (1 - \eta\lambda_0 + \frac{1}{5}\lambda_0\eta + O\left(\frac{\lambda_0\eta}{\sqrt{n}}\right) + \eta^2 n^2) \|y - u(k)\|_2^2 \]
\[\leq (1 - \eta\lambda_0 + \frac{1}{5}\lambda_0\eta + O\left(\frac{\lambda_0\eta}{\sqrt{n}}\right) + \frac{1}{5}\lambda_0\eta) \|y - u(k)\|_2^2 \]
\[\leq (1 - \frac{\eta\lambda_0}{2}) \|y - u(k)\|_2^2 , \] (78)
where \( I_2 := (I_2^1, ..., I_2^n)^\top \), (a) follows from (77), (72), (75), and (76), (b) follows from the fact that \( R := \frac{c\delta\lambda_0}{n^2} \) can be less than \( \frac{\delta\lambda_0}{n^2} \) by properly setting \( c \), and (c) follows from the definition of step size \( \eta = O\left(\frac{\lambda_0}{\sqrt{n}}\right) \) (i.e., \( \eta \) can be set less than \( \lambda_0/(5n^2) \)). We can rescale \( \delta \) to a constant such that the following condition (79) holds with probability at least \( 1 - \delta \) over the random initialization of \((W(0), a)\).
\[ \|y - u(k+1)\|_2^2 \leq (1 - \frac{\eta\lambda_0}{2}) \|y - u(k)\|_2^2 \] (79)

Therefore, by using the induction hypothesis with (79), with probability at least \( 1 - \delta \), it follows that for \( k \in \{0, 1, 2, ...\} \),
\[ \|y - u(k)\|^2 \leq (1 - \frac{\eta\lambda_0}{2})^k \|y - u(0)\|^2 . \] (80)

\[ \square \]

### A.5 Proof of Theorem 2.3

In this section, we prove Theorem 2.3. We first show some technical lemmas.

The following lemma (i.e., Lemma A.8) gives an upper bound of the gap between each trained weight vector and its initialization. This is the result of fixing \( \kappa \) in Lemma C.1 in [1] as \( \kappa = \Theta(1) \).
Lemma A.8 [Specific case of Lemma C.1 in [1] and Corollary of Lemma A.3]. Under same setting as Theorem A.2, i.e., \( \kappa = \Theta(1) \) for \( n \), \( \| y \| = O(\sqrt{n}) \), \( m = \Omega\left(\max\left(\frac{n^6}{\lambda_0^2 \sigma^2}, \frac{n^2}{\lambda_0} \log\left(\frac{2}{\delta}\right)\right)\right) \), set \( \{x_j\}_{j=1}^n \) of \( n \) training input samples is bounded as \( \max_{j \in \{n\}} \| x_j \| \leq 1 \), \( \eta = O\left(\frac{\lambda_0}{n^2}\right) \), and \( \lambda_0 = O(n^\gamma) > 0 \) with a constant \( \gamma \leq 1 \), it follows that with probability at least \( 1 - \delta \) over the random initialization of \( (W(0), a) \),

\[
\| w_r(k) - w_r(0) \| \leq 4\sqrt{n} \| y - u(0) \| \sqrt{\frac{m}{\lambda_0}} \leq O\left(\frac{\kappa n}{\sqrt{m \lambda_0 \delta}}\right) =: R
\]

(81)

Proof of Lemma A.8. The condition (37) is satisfied if the conditions in Theorem A.2 hold. Then, the proof is completed by combing Lemma A.3 and the fact that \( \| y - u(0) \| = O(\frac{\sqrt{n}}{\sqrt{\delta}}) \) holds with probability at least \( 1 - \delta \) (which is obtained from Lemma A.2 and the assumption \( \kappa = \Theta(1) \)).

The following lemma (i.e., Lemma A.9) is the result of fixing \( \kappa \) in Lemma C.2 in [1] as \( \kappa = \Theta(1) \). Therefore, we omit the proof of Lemma A.9 as Lemma A.9 is a specific case of Lemma C.2 in [1].

Lemma A.9 [Specific case of Lemma C.2 in [1]]. Under same setting as Theorem A.2, i.e., \( \kappa = \Theta(1) \) for \( n \), \( \| y \| = O(\sqrt{n}) \), \( m = \Omega\left(\max\left(\frac{n^6}{\lambda_0^2 \sigma^2}, \frac{n^2}{\lambda_0} \log\left(\frac{2}{\delta}\right)\right)\right) \), \( m = \Omega\left(\frac{n^6}{\lambda_0^2 \sigma^2}\right) \), set \( \{x_j\}_{j=1}^n \) of \( n \) training input samples is bounded as \( \max_{j \in \{n\}} \| x_j \| \leq 1 \), \( \eta = O\left(\frac{\lambda_0}{n^2}\right) \), and \( \lambda_0 = O(n^\gamma) > 0 \) with a constant \( \gamma \leq 1 \), it follows that with probability at least \( 1 - 4\delta \) over the random initialization, for all \( k \geq 0 \) we have

\[
\| H(k) - H(0) \| = O\left(\frac{n^3}{\sqrt{m \lambda_0 \delta^{3/2}}}\right),
\]

(82)

\[
\| Z(k) - Z(0) \| = O\left(\sqrt{\frac{n^2}{m \lambda_0 \delta^{3/2}}}\right).
\]

We also introduce Lemma C.3 in [1] as follows.

Lemma A.10 [Lemma C.3 in [1]]. With probability at least \( 1 - \delta \), we have \( \| H^\ast - H(0) \| = O\left(\frac{n^{\sqrt{\log(n/\delta)}}}{\sqrt{m}}\right) \).

Then, by using the above lemmas, we prove the following proposition. This result is a revision of Theorem 4.1 in [1] by removing a \( \kappa \)-affected value (i.e., \( (1 - \eta \lambda_0) \frac{k \sqrt{n}}{\sqrt{\delta}} \)) in the original bound given as in (33) in [1]. Therefore, this proposition is our major contribution to prove Theorem 2.3.

Proposition 7 (Modification/revision of Theorem 4.1 in [1]). Under same setting as Theorem A.2, i.e., \( \kappa = \Theta(1) \) for \( n \), \( \| y \| = O(\sqrt{n}) \), \( m = \Omega\left(\max\left(\frac{n^6}{\lambda_0^2 \sigma^2}, \frac{n^2}{\lambda_0} \log\left(\frac{2}{\delta}\right)\right)\right) \), set \( \{x_j\}_{j=1}^n \) of \( n \) training input samples is bounded as \( \max_{j \in \{n\}} \| x_j \| \leq 1 \), \( \eta = O\left(\frac{\lambda_0}{n^2}\right) \), and \( \lambda_0 = O(n^\gamma) > 0 \) with a constant \( \gamma \leq 1 \), it follows with probability at least \( 1 - \delta \) over the random initialization of \( (W(0), a) \) that for all \( k \in \{0, 1, \ldots\} \),

\[
 u(k) - y = -(I - \eta H^\ast)^k y + e(k),
\]

(83)

where

\[
\| e(k) \| = O\left(k \left(1 - \frac{\eta \lambda_0}{4}\right)^{k-1} \left(\frac{\eta n^{7/2}}{\sqrt{m \lambda_0 \delta^2}}\right)\right).
\]

(84)
Proof of Proposition 7. We define \( u_q(k) := f_{W(k)}(x_q) \) as the \( q \)th entry of \( u(k) := (f_{W(k)}(x_1), ..., f_{W(k)}(x_n))^\top \). Then,
\[
u_q(k+1) - \nu_q(k) = \frac{1}{\sqrt{m}} \sum_{r=1}^{m} a_r[\sigma(w_r(k+1)^\top x_q) - \sigma(w_r(k)^\top x_q)].\quad (85)
\]

We define the event
\[
A_{qr} := \{|w_r(0)^\top x_q| \leq R\},
\]
where \( R = O(\frac{m}{\sqrt{m\lambda_0\sqrt{\delta}}} \). Let \( S_q := \{ r \in \{1 : m \} : 1 \{A_{qr}\} = 0 \} \) and \( S_q^\perp := \{1 : m\} \setminus S_q \).

Note that \( w_r(0)^\top x_q \) has the same distribution as \( \mathcal{N}(0, \kappa^2) \) so that
\[
\mathbb{E}(1\{A_{qr}\}) = P_{h \sim \mathcal{N}(0, \kappa^2)}(|h| \leq R) = \int_{-R}^{R} \frac{1}{\sqrt{2\pi\kappa}}e^{-x^2/2\kappa^2}dx \leq \frac{2R}{\sqrt{2\pi\kappa}}.
\]

Then,
\[
\mathbb{E}(|S_q^\perp|) = \mathbb{E}(\sum_{r=1}^{m} 1\{A_{qr}\}) \leq \frac{2mR}{\sqrt{2\pi \kappa}}
\]
and
\[
\mathbb{E}(\sum_{q=1}^{n} |S_q^\perp|) = \mathbb{E}(\sum_{q=1}^{n} \sum_{r=1}^{m} 1\{A_{qr}\}) \leq \frac{2mnR}{\sqrt{2\pi \kappa}} = O(\frac{n^2 \sqrt{m}}{\lambda_0 \delta^{3/2}}),
\]

By Markov’s inequality with probability at least \( 1 - \delta \) over the random initialization of \((W(0), a)\),
\[
\sum_{q=1}^{n} |S_q^\perp| = O(\frac{n^2 \sqrt{m}}{\lambda_0 \delta^{3/2}}) \quad (86)
\]

From (85), we get
\[
u_q(k+1) - \nu_q(k) = \frac{1}{\sqrt{m}} \sum_{r \in S_q} a_r[\sigma(w_r(k+1)^\top x_q) - \sigma(w_r(k)^\top x_q)]
\]
\[
+ \frac{1}{\sqrt{m}} \sum_{r \in S_q^\perp} a_r[\sigma(w_r(k+1)^\top x_q) - \sigma(w_r(k)^\top x_q)] \quad (87)
\]
We denote the second term as $\dot{\epsilon}_q(k)$

$$|\dot{\epsilon}_q(k)| = \left| \frac{1}{\sqrt{m}} \sum_{r \in S_q^\perp} a_r [\sigma(w_r(k+1)^\top x_q) - \sigma(w_r(k)^\top x_q)] \right|$$

$$\leq \frac{1}{\sqrt{m}} \sum_{r \in S_q^\perp} \|w_r(k+1) - w_r(k)\|$$

$$= \frac{\eta}{\sqrt{m}} \sum_{r \in S_q^\perp} \left\| \frac{\partial L_i(W(k))}{\partial w_r(k)} \right\|$$

$$\leq \frac{\eta}{m} \sum_{r \in S_q^\perp} \sum_{j=1}^n |y_j - u_j(k)|$$

$$\leq \frac{\eta \sqrt{n|S_q^\perp|}}{m} \|y - u(k)\|. \quad (88)$$

For the first term in (87),

$$\frac{1}{\sqrt{m}} \sum_{r \in S_q} a_r [\sigma(w_r(k+1)^\top x_q) - \sigma(w_r(k)^\top x_q)]$$

$$= \frac{1}{\sqrt{m}} \sum_{r \in S_q} a_r \{w_r(k)^\top x_q \geq 0\} (w_r(k+1) - w_r(k))^\top x_q$$

$$= \frac{1}{\sqrt{m}} \sum_{r \in S_q} a_r \{w_r(k)^\top x_q \geq 0\} (-\frac{\eta}{\sqrt{m}} \sum_{p=1}^n (u_p(k) - y_p) a_r x_q \{w_r(k)^\top x_p \geq 0\})^\top x_q$$

$$= -\frac{\eta}{m} \sum_{p=1}^n (u_p(k) - y_p) x_p^\top x_q \sum_{r \in S_q} \{w_r(k)^\top x_p \geq 0\} \{w_r(k)^\top x_q \geq 0\} + \bar{\epsilon}_q(k)$$

$$= -\eta \sum_{p=1}^n (u_p(k) - y_p) H_{qp}(k) + \bar{\epsilon}_q(k), \quad (89)$$

where

$$\bar{\epsilon}_q(k) = \frac{\eta}{m} \sum_{p=1}^n (u_p(k) - y_p) x_p^\top x_q \sum_{r \in S_q^\perp} \{w_r(k)^\top x_p \geq 0\} \{w_r(k)^\top x_q \geq 0\}. \quad (90)$$

Then,

$$|\bar{\epsilon}_q(k)| \leq \frac{\eta \sqrt{n|S_q^\perp|}}{m} \|y - u(k)\|. \quad (91)$$

Combining (87), (88), (89) and (91),

$$u_q(k+1) - u_q(k) = -\eta \sum_{p=1}^n (u_p(k) - y_p) H_{qp}(k) + \dot{\epsilon}_q(k) + \bar{\epsilon}_q(k) \quad (92)$$
which gives
\[ u(k+1) - u(k) = -\eta H(k)(u(k) - y) + \epsilon(k), \]  
(93)
where \( \epsilon(k) = \dot{\epsilon}(k) + \bar{\epsilon}(k) \). Note that by using (86),
\[ \|\epsilon(k)\| \leq \|\epsilon(k)\|_1 = \sum_{q=1}^{n} |\epsilon_q(k) + \bar{\epsilon}_q(k)| \leq \sum_{q=1}^{n} \frac{2\eta \sqrt{n}|S_q^k|}{m} \|y - u(k)\| = O\left(\frac{\eta m^{5/2}}{\sqrt{m\lambda_0} \delta^{3/2}}\right) \|y - u(k)\|. \]  
(94)

We rewrite (93) as
\[ u(k+1) - u(k) = -\eta H^*(u(k) - y) + \zeta(k), \]  
(95)
where \( \zeta(k) = \eta(H^* - H(k))(u(k) - y) + \epsilon(k) \). Then, we get
\[ u(k) - y = -(1 - \eta H^*)^k(y - u(0)) + \sum_{t=0}^{k-1} (I - \eta H^*)^t \zeta(k - 1 - t). \]  
(96)

From (94) and Lemmas A.9 and A.10, we bound \( \zeta(k) \) as
\[ \|\zeta(k)\| \leq \eta \|H^* - H(k)\| \|y - u(k)\| + O\left(\frac{\eta m^{5/2}}{\sqrt{m\lambda_0} \delta^{3/2}}\right) \|y - u(k)\| \]
\[ \leq \eta(\|H^*(0) - H(0)\| + \|H^* - H(0)\|) \|y - u(k)\| + O\left(\frac{\eta m^{5/2}}{\sqrt{m\lambda_0} \delta^{3/2}}\right) \|y - u(k)\| \]
\[ = O\left(\frac{\eta m^{3}}{\sqrt{m\lambda_0} \delta^{3/2}} + \frac{\eta \sqrt{\log(n/\delta)}}{\sqrt{m}} + \frac{\eta m^{5/2}}{\sqrt{m\lambda_0} \delta^{3/2}}\right) \|y - u(k)\| \]
\[ = O\left(\frac{\eta m^{3}}{\sqrt{m\lambda_0} \delta^{3/2}}\right) \|y - u(k)\|, \]  
(97)
where the last equality follows from the fact that \( O\left(\frac{\eta m^{3}}{\sqrt{m\lambda_0} \delta^{3/2}}\right) \) implies \( O\left(\frac{\eta m^{5/2}}{\sqrt{m\lambda_0} \delta^{3/2}}\right) \) and \( O\left(\frac{\eta \sqrt{\log(n/\delta)}}{\sqrt{m}}\right) \).  

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Then,
\[
\left\| \sum_{t=0}^{k-1} (I - \eta H^*)^t \zeta(k-1-t) \right\| \leq \sum_{t=0}^{k-1} \| I - \eta H^* \|^t \| \zeta(k-1-t) \|
\]
\[
\leq \sum_{t=0}^{k-1} \| I - \eta H^* \|^t \| \zeta(k-1-t) \|
\]
\[
\leq \sum_{t=0}^{k-1} (1 - \eta \lambda_0)^t \| \zeta(k-1-t) \|
\]
\[
\leq \sum_{t=0}^{k-1} (1 - \eta \lambda_0)^t O\left(\frac{m^3}{\sqrt{m \lambda_0 \delta^{3/2}}}\right) \| y - u(k-1-t) \|
\]
\[
\leq k (1 - \frac{\eta \lambda_0}{4})^{k-1} O\left(\frac{n^{7/2}}{\sqrt{m \lambda_0 \delta^{2}}}\right),
\]  
(98)

where (a) follows from (97), (b) follows from Theorem A.2 such that
\[
\| y - u(k) \| \leq (1 - \frac{\eta \lambda_0}{2})^{k/2} \| y - u(0) \| \leq (1 - \frac{\eta \lambda_0}{4})^k \| y - u(0) \|,
\]  
(99)

and (c) follows from Lemma A.2 and the assumption \( \kappa = \Theta(1) \) (i.e., \( \| y - u(0) \| = O\left(\frac{n^{1/2}}{\sqrt{\delta}}\right) \)).

By applying (98) to (96), it follows that under same setting as Theorem A.2, it follows that for \( k \geq 0 \), with probability at least \( 1 - \delta \),
\[
u(k) - y = -(I - \eta H^*)^k (y - u(0)) + e(k),
\]  
(100)

where
\[
\| e(k) \| = O\left( k \left(1 - \frac{\eta \lambda_0}{4}\right)^{k-1} \left(\frac{n^{7/2}}{\sqrt{m \lambda_0 \delta^{2}}}\right)\right).
\]  
(101)

As a simple corollary of Proposition 7, now we can prove Theorem 2.3 as follows.

**Theorem A.3.** ([Theorem 2.3, modification/revision of Theorem 4.1 in [1]] Suppose that all conditions in Theorem 2.1 hold. Suppose also that \( \kappa = \Theta(1) \). Then, with probability at least \( 1 - \delta \) for \( \delta \in (0, 1) \) over the random initialization of \((W(0), a)\), it follows that for all \( k \geq 0 \),
\[
\frac{1}{\sqrt{n}} \| y - u(k) \| = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (1 - \eta \lambda_i)^{2k} \left( v_i^T (y - u(0)) \right)^2} + O\left(\frac{n^3}{\sqrt{m \lambda_0^2 \delta^2}}\right),
\]  
(102)

where \( v_1, ..., v_n \in \mathbb{R}^n \) are orthonormal eigenvectors of \( H^* \) and \( \lambda_1, ..., \lambda_n \) are the corresponding eigenvalues.
Proof of Theorem A.3. Our proof is based on that for Theorem 4.1 in [1]. From Proposition 7, it follows that for all $k \in \{0, 1, \ldots\}$,

$$u(k) - y = -(I - \eta H^*)^k y + e(k), \quad (103)$$

where

$$\|e(k)\| = O\left(k \left(1 - \frac{\eta \lambda_0}{4}\right)^{k-1} \left(\frac{\eta n^{7/2}}{\sqrt{m \lambda_0 \delta^2}}\right)\right). \quad (104)$$

Therefore, we get

$$\|u(k) - y\| \leq \left(\sum_{j=1}^{n} (1 - \eta \lambda_j)^{2k} (v_j^\top (y - u(0)))^2 + \|e(k)\|\right)^{\frac{1}{n}} \leq \left(\sum_{j=1}^{n} (1 - \eta \lambda_j)^{2k} (v_j^\top (y - u(0)))^2 + O\left(k \left(1 - \frac{\eta \lambda_0}{4}\right)^{k-1} \frac{\eta n^{7/2}}{\sqrt{m \lambda_0 \delta^2}}\right)\right)^{\frac{1}{n}} \leq \left(\sum_{j=1}^{n} (1 - \eta \lambda_j)^{2k} (v_j^\top (y - u(0)))^2 + O\left(\frac{1}{\eta \lambda_0} \frac{\eta n^{7/2}}{\sqrt{m \lambda_0 \delta^2}}\right)\right)^{\frac{1}{n}}, \quad (105)$$

where (a) follows from the triangle inequality and (103), (b) follows from $(I - \eta H^*)^k$ has the eigen-decomposition $(I - \eta H^*)^k = \sum_{j=1}^{n} (1 - \eta \lambda_j)^{k} v_j v_j^\top$ and $y - u(0)$ can be decomposed as $y - u(0) = \sum_{j=1}^{n} (v_j^\top (y - u(0)))v_j$, (c) follows from (104), (d) follows from $\max_{k \geq 0} \{k (1 - \eta \lambda_0/4)^{k-1}\} = O(1/(\eta \lambda_0)).$ \hfill \qed

A.6 Proof of Theorem 2.4

A.6.1 Background on Rademacher Complexity

Before we prove Theorem 2.4 stated in Section 2.3, we introduce Rademacher Complexity and the theorem derived from it.

Define a loss function $\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$. For a function $f : \mathbb{R}^d \to \mathbb{R}$, we define the population loss over true model distribution $\mathcal{D}$ and the empirical loss over $n$ samples $S = \{(x_j, y_j)\}_{j=1}^{n}$ from $\mathcal{D}$, respectively, as

$$\mathcal{L}_D(f) = \mathbb{E}_{(x,y) \sim \mathcal{D}}[\ell(f(x), y)]$$ $$\mathcal{L}_S(f) = \frac{1}{n} \sum_{j=1}^{n} \ell(f(x_j), y_j). \quad (105)$$

Then, Rademacher complexity of a function class $\mathcal{F}$ mapping $\mathbb{R}^d$ to $\mathbb{R}$ is expressed as

$$\mathcal{R}_S(\mathcal{F}) := \frac{1}{n} \mathbb{E}_{\epsilon} \left[\sup_{f \in \mathcal{F}} \sum_{j=1}^{n} \epsilon_j f(x_j)\right], \quad (106)$$

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Then, with probability at least \( 1 - \delta \) over sample \( S \) of size \( n \),
\[
\sup_{f \in \mathcal{F}} \{ \mathcal{L}_{D}(f) - \mathcal{L}_{S}(f) \} \leq 2\alpha \mathcal{R}_{S}(\mathcal{F}) + 3\beta \sqrt{\frac{\log(2/\delta)}{2n}}.
\] (107)

A.6.2 Proof of Theorem 2.4

In this section, we now prove Theorem 2.4 stated in Section 2.3. We first show some technical lemmas.

As a result of Lemma A.8, we can obtain the following upper bound of the magnitude of trained NN output, when the neural network is over-parameterized.

**Lemma A.11.** Let the input data \( \{x_j\}_{j=1}^{n} \) and label data \( \{y_j\}_{j=1}^{n} \) of \( n \) training samples independently follow model distribution \( D(x, y) \). We consider the same setting as Theorem A.2, i.e., \( \kappa = \Theta(1) \) for \( n \), \( \|y\| = O(\sqrt{n}) \), \( m = \Omega\left(\max\left(\frac{n^6}{\lambda_0^2 \kappa^2 \beta^2}, \frac{n^2}{\lambda_0^2} \log^2(\frac{n}{\delta})\right)\right) \), set \( \{x_j\}_{j=1}^{n} \) of \( n \) training input samples is bounded as \( \max_{j \in \{n\}} \|x_j\| \leq 1 \), \( \eta = O\left(\frac{\lambda_0}{n^\gamma}\right) \), and \( \lambda_0 = O(n^\gamma) > 0 \) with a constant \( \gamma \leq 1 \). Then, for input sample \( x \) obtained from \( D(x, y) \) and for every \( k \geq 0 \), it follows that with probability at least \( 1 - \delta \) over the random initialization of \( (W(0), \mathbf{a}) \),
\[
|f_{W(k), \mathbf{a}}(x)| = O\left(\frac{K}{\delta}\right).
\] (108)

**Proof of Lemma A.11.** The proof is similar with that for Lemma A.4. Define a set \( \Gamma(W(0), R') := \left\{ W = [\hat{w}_1, ..., \hat{w}_m] \in \mathbb{R}^{m \times d} \mid \max_{r \in \{m\}} \|\hat{w}_r - w_r(0)\| \leq R' \right\} \). Then, for any matrix \( W = [\hat{w}_1, ..., \hat{w}_m] \in \mathbb{R}^{m \times d} \) belonging to \( \Gamma(W(0), R') \), it follows that for any \( x \in \mathbb{R}^d \),
\[
\mathbb{E}_a[f_{W}(x)^2] = \mathbb{E}_a\left[ \frac{1}{m} \left( \sum_{r \in \{m\}} a_r \sigma(\hat{w}_r^\top x) \right)^2 \right]
= \mathbb{E}_a\left[ \frac{1}{m} \left( \sum_{r \in \{m\}} \sigma(\hat{w}_r^\top x)^2 + \sum_{r, r' \in \{m\} \times \{m\}, r \neq r'} a_r a_{r'} \sigma(\hat{w}_r^\top x) \sigma(\hat{w}_{r'}^\top x) \right) \right]
= \frac{1}{m} \left( \sum_{r \in \{m\}} \sigma(\hat{w}_r^\top x)^2 \right) + \frac{1}{m} \left( \sum_{r, r' \in \{m\} \times \{m\}, r \neq r'} \mathbb{E}_a[a_r a_{r'}] \sigma(\hat{w}_r^\top x) \sigma(\hat{w}_{r'}^\top x) \right)
= \frac{1}{m} \left( \sum_{r \in \{m\}} \sigma(\hat{w}_r^\top x)^2 \right),
\] (109)

where (a) follows from \( \hat{w}_r \) and \( \hat{w}_{r'} \) are independent of the random vector \( \mathbf{a} \) (i.e., \( \hat{w}_r \) and \( \hat{w}_{r'} \) are only depending on \( W(0) \) and \( R' \) as \( W \) is an arbitrary matrix satisfying \( W \in \Gamma(W(0), R') \)). Thus, by using Markov’s inequality, we obtain with probability at least \( 1 - \delta \) over the random initialization of \( \mathbf{a} \),
\[
|f_{W}(x)| \leq \frac{1}{\delta m} \sum_{r=1}^{m} \sigma(\hat{w}_r^\top x)^2.
\] (110)
Using (110), the following inequalities hold with probability at least $1 - \Omega(\delta)$ over the random initialization of $(W(0), a)$,

$$f_W(x)^2 \leq \frac{1}{\delta m} \sum_{r=1}^{m} \sigma((\tilde{w}_r - w_r(0) + w_r(0))^\top x)^2$$

$$\leq \frac{1}{\delta m} \sum_{r=1}^{m} (\|\tilde{w}_r - w_r(0)\|^2) + \frac{1}{\delta m} \sum_{r=1}^{m} \|w_r(0)^\top x\| \|x\|$$

$$(b) \leq \frac{R^2}{\delta} + \frac{1}{\delta m} \sum_{r=1}^{m} \|w_r(0)^\top x\| \|x\|$$

$$(c) \leq \frac{R^2}{\delta} + \frac{1}{\delta m} \sum_{r=1}^{m} \|w_r(0)\|^2$$

$$(d) \leq \frac{R^2}{\delta} + \frac{\kappa^2}{\delta^2},$$

(111)

where (a) follows from (110), (b) follows from the fact that $\tilde{W}$ belongs to $\Gamma(W(0), R)$ (i.e., $\|\tilde{w}_r - w_r(0)\| \leq R$), (c) follows from Cauchy–Schwarz inequality, and (d) follows from the fact that $\mathbb{E}[\sum_{r=1}^{m} \|w_r(0)\|^2] = m\kappa^2$ and Markov’s inequality (i.e., $\sum_{r=1}^{m} \|w_r(0)\|^2 = m\kappa^2/\delta$ holds with probability at least $\delta$).

On the other hand, it follows from Lemma A.8 that $W(k)$ belongs to $\Gamma(W(0), R')$ with probability at least $1 - \delta$ over the random initialization of $(W(0), a)$, where $R' = \sqrt{\frac{c\kappa^2n^2}{m\lambda_0\delta^2}}$ for some constant $c$. This implies $\tilde{W}$ in (111) can be replaced by $W(k)$ (i.e., $f_W(x)$ in (111) can be replaced by $f_W(k)(x)$).

By using the union bound over the above statement (i.e., $f_W(x)$ in (111) can be replaced by $f_W(k)(x)$) and the inequality in (111) and setting $R' = \sqrt{\frac{c\kappa^2n^2}{m\lambda_0\delta^2}}$, it follows that with probability at least $1 - \Omega(\delta)$ over the random initialization of $(W(0), a)$,

$$|f_W(k)_a(x)|^2 \leq \frac{1}{\delta} \left( \frac{\kappa n}{\sqrt{m\lambda_0\delta}} \right)^2 + \frac{\kappa^2}{\delta^2}$$

$$\leq \frac{1}{\delta} \left( \frac{\kappa^2}{\delta^2} \right),$$

(112)

The proof is completed by rescaling $\delta$ to a constant such that (112) holds with probability at least $1 - \delta$.

We can obtain the following lemma A.12 by modifying Lemma 5.3 in [1]. Note that Lemma 5.3 in [1] provides an upper bound of distance between trained NN weights and its initial ones. Lemma A.12 is a result obtained by removing the terms affected by $\kappa$ from this upper bound of Lemma 5.3 in [1]. Therefore, this lemma is our major contribution to prove Theorem 2.4.

**Lemma A.12** [Modification/revision of Lemma 5.3 in [1]]. Consider the same setting as Theorem A.2, i.e., $\kappa = \Theta(1)$ for $n$, $\|y\| = O(\sqrt{n})$, $m = \Omega\left(\max\left(\frac{b^6}{\lambda_0^2\alpha^2}, \frac{a^2}{\lambda_0^2} \log(\frac{n}{\eta})\right)\right)$, set $\{x_j\}_{j=1}^n$ of $n$ training input samples is bounded as $\max_{j \in [n]} \|x_j\| \leq 1$, $\eta = O(\frac{\lambda_0}{\alpha})$, and $\lambda_0 = O(n^{\gamma}) > 0$ with a constant $\gamma \leq 1$. Then, with probability at least $1 - \delta$ over the random initialization of $(W(0), a)$, it follows that for all $k \geq 0$
\( \| w_r(k) - w_r(0) \| = O \left( \frac{k n}{\sqrt{m \lambda_0 \delta}} \right) (:= R), \forall r \in \{1 : m\} \)

\( \| W(k) - W(0) \| \leq \sqrt{\| y - u(0) \| (H^*)^{-1}(y - u(0))} + O \left( \sqrt{\frac{n^2 \sqrt{\log(n/\delta)}}{\lambda_0 \sqrt{m}} + \sqrt{\frac{n^2}{m \lambda_0^{3/2}} + \frac{n^4}{m \lambda_0^{3/2}}} \right) \)

**Proof of Lemma A.12.** The first part is proved by using Lemma A.8. The rest is to prove the second part.

From Proposition 7, we get
\[
 u(k) - y = -(I - \eta H^* )^k (y - u(0)) + e(k), \tag{113}
\]
where
\[
 \| e(k) \| = O \left( k \left( 1 - \frac{\eta \lambda_0}{4} \right) k^{-1} \left( \frac{\eta n^{7/2}}{\sqrt{m \lambda_0 \delta^2}} \right) \right). \tag{114}
\]

We apply (113) to (26), which is
\[
 \text{vec}(W(k+1)) = \text{vec}(W(k)) - \eta Z(k)(u(k) - y), \tag{115}
\]
and for \( k \in \{0, ..., K - 1 \} \) we obtain
\[
 \begin{align*}
 \text{vec}(W(k)) - \text{vec}(W(0)) \\
 = - \sum_{k=0}^{K-1} \eta Z(k)(u(k) - y) \\
 = \sum_{k=0}^{K-1} \eta Z(k)((I - \eta H^*)^k (y - u(0)) - e(k)) \\
 = \sum_{k=0}^{K-1} \eta Z(0)(I - \eta H^*)^k (y - u(0)) + \sum_{k=0}^{K-1} \eta (Z(k) - Z(0))(I - \eta H^*)^k (y - u(0)) - \sum_{k=0}^{K-1} \eta Z(k)e(k). \tag{116}
\end{align*}
\]

Then we bound the first term of (116) as
\[
\begin{align*}
 \left\| \sum_{k=0}^{K-1} \eta Z(0)(I - \eta H^*)^k (y - u(0)) \right\|^2 \\
 = \| Z(0) T(y - u(0)) \|^2 \\
 = (y - u(0))^\top T H(0) T(y - u(0)) \\
 \leq (y - u(0))^\top T H^* T(y - u(0)) + \| H^* - H(0) \|_2 \| y - u(0) \|^2 \| T \|^2 \\
 \overset{(a)}{=} (y - u(0))^\top T H^* T(y - u(0)) + O \left( \frac{n \sqrt{\log(n/\delta)}}{\sqrt{m}} \right) \left( \frac{n}{\delta} \right) \left( \frac{1}{\lambda_0} \right)^2 \\
 = (y - u(0))^\top T H^* T(y - u(0)) + O \left( \frac{n^2 \sqrt{\log(n/\delta)}}{\delta \lambda_0^{3/2}} \sqrt{m} \right),
\end{align*}
\]

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where $T := \sum_{i=1}^{n} \sum_{k=0}^{K-1} \eta(1 - \eta \lambda_i)^k v_i v_i^\top = \sum_{i=1}^{n} \frac{1 - (1-\eta \lambda_i)^K}{\lambda_i} v_i v_i^\top \ (v_1, ..., v_n \in \mathbb{R}^n$ are orthonormal eigenvectors of $H^*$ and $\lambda_1, ..., \lambda_n$ are the corresponding eigenvalues) and (a) follows from Lemma A.10 and Lemma A.2. Then,

$$
\sum_{k=0}^{K-1} \eta Z(0)(I - \eta H^*)^k(y - u(0)) \leq \sqrt{(y - u(0))^\top T H^* T (y - u(0)) + O\left(\frac{n^2 \sqrt{\log(n/\delta)}}{\lambda_0^2 \sqrt{m}}\right)}.
$$

By using

$$
TH^* T = \sum_{i=1}^{n} \left(\frac{1 - (1 - \eta \lambda_i)^K}{\lambda_i}\right)^2 \lambda_i v_i v_i^\top \leq \sum_{i=1}^{n} \frac{1}{\lambda_i} v_i v_i^\top = (H^*)^{-1},
$$

we get

$$
\sum_{k=0}^{K-1} \eta Z(0)(I - \eta H^*)^k(y - u(0)) \leq \sqrt{(y - u(0))^\top (H^*)^{-1} (y - u(0)) + O\left(\frac{n^2 \sqrt{\log(n/\delta)}}{\lambda_0^2 \sqrt{m}}\right)}.
$$

We bound the second term of (116) as

$$
\sum_{k=0}^{K-1} \eta^* Z(0)(1 - \eta H^*)^k(y - u(0)) \leq \eta \sum_{k=0}^{K-1} \eta \|Z(k) - Z(0)\|_2 \|I - \eta H^*\|^k \|y - u(0)\|_2
$$

$$
\leq \eta \sum_{k=0}^{K-1} \|Z(k) - Z(0)\|_2 \|I - \eta H^*\|^k \|y - u(0)\|_2
$$

$$
\leq \eta \|Z(k) - Z(0)\|_2 \sum_{k=0}^{K-1} (1 - \eta \lambda_0)^k \|y - u(0)\|_2
$$

$$
= O\left(\sqrt{\frac{n^2}{\sqrt{m} \lambda_0^3/2}}\right) \sum_{k=0}^{K-1} \eta(1 - \eta \lambda_0)^k \|y - u(0)\|_2
$$

$$
\leq O\left(\sqrt{\frac{n^3}{\sqrt{m} \lambda_0^3/2}}\right),
$$

where (a) follows from Lemma A.9 and (b) follows from $\sum_{k=0}^{K-1} \eta(1 - \eta \lambda_0)^k = \frac{1 - (1-\eta \lambda_0)^K}{\lambda_0} \leq \frac{1}{\lambda_0}$. 

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By using (114) and the fact that \( \|Z(k)\| \leq \sqrt{n} \), we bound the third term of (116) as

\[
\left\| \sum_{k=0}^{K-1} \eta Z(k)e(k) \right\| = O\left( \sum_{k=0}^{K-1} \eta \sqrt{n} \cdot \left[ k \left( 1 - \frac{\eta \lambda_0}{4} \right)^{k-1} \left( \frac{\eta n^{7/2}}{\sqrt{m \lambda_0 \delta^2}} \right) \right] \right)
\]

\[
= O\left( \sum_{k=0}^{K-1} k \left( 1 - \frac{\eta \lambda_0}{4} \right)^{k-1} \left( \frac{\eta^2 n^4}{\sqrt{m \lambda_0 \delta^2}} \right) \right)
\]

\[
\overset{(a)}{=} O\left( \frac{n^4}{\sqrt{m \lambda_0 \delta^2}} \right),
\]

where (a) follows from the fact that \( \sum_{k=0}^{K-1} k \left( 1 - \frac{\eta \lambda_0}{4} \right)^{k-1} \leq \sum_{k=0}^{\infty} k \left( 1 - \frac{\eta \lambda_0}{4} \right)^{k-1} = \left( \frac{4 \eta \lambda_0}{\lambda_0} \right)^2 \).

Therefore, by applying (119), (120), and (121) to (116),

\[
\|W(k) - W(0)\|
\]

\[
\leq \sqrt{(y - u(0))^\top (H^*)^{-1} (y - u(0))} + O \left( \sqrt{\frac{n^2 \sqrt{\log(n/\delta)}}{\lambda_0 \sqrt{n}}} + \sqrt{\frac{n^3}{\sqrt{m \lambda_0 \delta^3/2}}} + \frac{n^4}{\sqrt{m \lambda_0 \delta^2}} \right)
\]

\[
\square
\]

We introduce the following lemma (i.e., Lemma A.13) proved by [1]. This lemma shows Rademacher complexity can be upper bounded by a term depending on the distance between the trained weight and its initial value.

**Lemma A.13** [Lemma 5.4 in [1]]. Given \( R > 0 \), we assume that the input data \( \{x_j\}_{j=1}^{n} \) is given as \( \|x_j\| \leq 1 \) for \( j \in \{n\} \). Consider the following function class in (122) with \( W(0) =: [w_1(0), \ldots, w_m(0)] \)

\[
\mathcal{F}^{W(0)}_{R,B} := \{ f_{W,a} : W = [\hat{w}_1, \ldots, \hat{w}_m] \}, \|\hat{w}_r - w_r(0)\| \leq R \left( \forall r \in \{m\} \right), \|\hat{W} - W(0)\| \leq B \}. \quad (122)
\]

Then it follows that with a probability at least 1 – \( \delta \) over the random initialization of \( (W(0), a) \), for every \( B > 0 \), the empirical Rademacher complexity \( R_S(\mathcal{F}^{W(0),a}_{R,B}) \) based on the function class in (122) is bounded as

\[
R_S(\mathcal{F}^{W(0),a}_{R,B}) := \frac{1}{n} \mathbb{E}_{\epsilon \in \{\pm 1\}^n} \left[ \sup_{f \in \mathcal{F}^{W(0),a}_{R,B}} \sum_{j=1}^{n} \epsilon_j f(x_j) \right]
\]

\[
\leq \frac{B}{\sqrt{2n}} \left( 1 + \left( \frac{2}{\sqrt{m}} \right)^{1/4} \right) + \frac{2R^2 \sqrt{n}}{\kappa} + R \sqrt{2 \log \frac{2}{\delta}}.
\]

Now, by using Lemmas A.8, A.11, and A.13, we prove Theorem 2.4, which is given as Theorem A.5.

**Theorem A.5.** [Theorem 2.4, modification/revision of Theorem 5.1 in [1]] Suppose that all conditions except \( \lambda_0 > 0 \) in Theorem 2.1 hold and we fix a failure probability \( \delta \in (0, 1) \). Suppose further that \( \kappa = \Theta(1) \) and \( m = \Omega(\log(n, \lambda_0^{-1}, \delta^{-1})) \). Suppose also that \( \lambda_0 > 0 \) holds with probability at least \( 1 - \delta/3 \) for \( n \) i.i.d. training samples \( \{(x_i, y_i)\}_{i=1}^{n} \) from true model distribution \( D \). Then, with
We also assume the following conditions hold: κ

Proof of Theorem A.5. We consider a loss function ℓ(a, b) : ℝ × ℝ → ℝ as ℓ(a, b) = (a - b)²/2. We assume that this loss function ℓ(a, b) is α-Lipschitz in the first argument, this function is bounded in [0, β], and α and β follow O(1). We will prove that this assumption holds at the end of the proof.

Using the loss function and (105), we can define the population loss over true model distribution D and the empirical loss over n samples S, respectively, as

\[
\mathcal{L}_D(f) = \mathbb{E}_{(x, y) \sim D} [\ell(f(x), y)] = \mathbb{E}_{(x, y) \sim D} \left[ \frac{1}{2} (f(x) - y)^2 \right]
\]

\[
\mathcal{L}_S(f) = \sum_{j=1}^{n} [\ell(f(x_j), y_j)] = \sum_{j=1}^{n} \left[ \frac{1}{2} (f(x_j) - y_j)^2 \right],
\]

where \( f : \mathbb{R}^d \rightarrow \mathbb{R} \) denotes a trained neural network to be specified (i.e., \( f_{W(k)} \)).

We assume that \( \lambda_0 = O(n^\gamma) > 0 \) with a constant \( \gamma \leq 1 \) holds with probability at least 1 - δ/3. We also assume the following conditions hold: \( \kappa = \Theta(1) \) for \( n, \|y\| = O(\sqrt{n}) \), \( \eta = O(\frac{\lambda_0}{n}) \), and \( m = \Omega(\frac{n^6}{\delta^5}) \).

With probability at least 1 - δ/6 over the random initialization of \((W(0), a)\), the followings hold simultaneously:

- Optimization succeeds: By using Theorem A.2 with (64), and the fact that \( \|y - u(0)\| = O(\sqrt{n}) \) (which is obtained from Lemma A.2 and the assumption \( \kappa = \Theta(1) \)), if \( k = \Omega(\frac{1}{\eta \lambda_0} \log \frac{n}{\delta}) \), it follows that

\[
L(W(k)) \leq (1 - \frac{\eta \lambda_0}{2})^k O\left(\frac{n}{\delta}\right) \leq \frac{1}{2}.
\]

Then,

\[
\mathcal{L}_S(f_{W(k)}) := \frac{1}{2n} \sum_{q=1}^{n} |f_{W(k)}(x_q) - y_q|^2
\]

\[
= \frac{1}{n} L(W(k))
\]

\[
\overset{(a)}{=} O\left(\frac{1}{n}\right),
\]

where (a) follows from (125).

- From Lemma A.12, we get \( \|w_r(k) - w_r(0)\| = R \) (\( \forall r \in \{1 : m\} \)) where \( R = O\left(\frac{n}{\sqrt{m \lambda_0 \delta}}\right) \), and \( \|W(k) - W(0)\| \leq B \) where \( B = \sqrt{(y - u(0))^T (H^*)^{-1} (y - u(0))} + O\left(\sqrt{n^2 \log(n/\delta)} \frac{\lambda_0}{\lambda_0' \sqrt{m}} + \sqrt{\frac{n^4}{\sqrt{m \lambda_0' \delta^2}} + \frac{n^4}{\sqrt{m \lambda_0' \delta^2}}}ight) \). Note that \( B \leq O\left(\frac{n}{\lambda_0}\right) \).
Let $B_j = j (j = 1, 2, ...).$ For all $i$, the function class $F_{R,B_j}^{(0),a}$ has Rademacher complexity, which is upper bounded by

$$\mathcal{R}_S(F_{R,B_j}^{(0),a}) \leq \frac{B_j}{\sqrt{2n}} \left(1 + \left(\frac{2 \log \frac{20}{\delta}}{m}\right)^{1/4}\right) + \frac{2R^2\sqrt{m}}{\kappa} + R\sqrt{2 \log \frac{20}{\delta}} \quad (127)$$

Let $j^*$ be the smallest integer such that $B \leq B_{j^*}$. Then we have $B_{j^*} \leq B + 1$ and $j^* \leq O(\frac{n}{\lambda_0})$. Note that $f_{W(0),a} \in F_{R,B_j}^{(0),a}$. And we get

$$\mathcal{R}_S(F_{R,B_j}^{(0),a}) \leq \frac{B + 1}{\sqrt{2n}} \left(1 + \left(\frac{2 \log \frac{20}{\delta}}{m}\right)^{1/4}\right) + O(R^2\sqrt{m}) + R\sqrt{2 \log \frac{20}{\delta}}$$

$$= \frac{A}{\sqrt{2n}} \left(1 + \left(\frac{2 \log \frac{20}{\delta}}{m}\right)^{1/4}\right) + O\left(\frac{1}{\sqrt{n}}\right) + O\left(\frac{\text{poly}(n, \frac{1}{\lambda_0}, \frac{1}{\delta})}{m^{1/4}}\right) + O\left(\frac{\text{poly}(n, \frac{1}{\lambda_0}, \frac{1}{\delta})}{m^{1/4}}\right)$$

$$= \frac{A}{\sqrt{2n}} + O\left(\frac{1}{\sqrt{n}}\right) + O\left(\frac{\text{poly}(n, \frac{1}{\lambda_0}, \frac{1}{\delta})}{m^{1/4}}\right), \quad (128)$$

where $A = \sqrt{(y-u(0))^\top (H^*)^{-1} (y-u(0))}$. From the result of Rademacher complexity (Theorem A.4) and the union bound over a finite set $\{1 : B_{j^*}\}$, with probability at least $1 - \delta/6$, the following inequality holds for all $j \in \{1, 2, ..., j^*\}$.

$$\sup_{f \in F_{R,B_j}^{(0),a}} \{\mathcal{L}_D(f) - \mathcal{L}_S(f)\} \leq 2\alpha \mathcal{R}_S(F_{R,B_j}^{(0),a}) + O\left(\beta \sqrt{\frac{\log \left(\frac{n}{\lambda_0 \delta}\right)}{2n}}\right) \quad (129)$$

By using the union bound jointly to consider (126), (128), and (129), we obtain the fact that with probability at least $1 - 5\delta/6$, the followings are satisfied at the same time.

$$\mathcal{L}_S(f_{W(k),a}) = O\left(\frac{1}{n}\right)$$

$$f_{W(k),a} \in F_{R,B_j}^{(0),a}$$

$$\mathcal{R}_S(F_{R,B_j}^{(0),a}) = \sqrt{(y-u(0))^\top (H^*)^{-1} (y-u(0))} \frac{1}{2n} + O\left(\frac{1}{\sqrt{n}}\right) + O\left(\frac{\text{poly}(n, \frac{1}{\lambda_0}, \frac{1}{\delta})}{m^{1/4}}\right)$$

$$\sup_{f \in F_{R}^{(0),a}} \{\mathcal{L}_D(f) - \mathcal{L}_S(f)\} \leq 2\alpha \mathcal{R}_S(F_{R}^{(0),a}) + O\left(\beta \sqrt{\frac{\log \left(\frac{n}{\lambda_0 \delta}\right)}{2n}}\right) \quad (130)$$
If the assumption that $\alpha$ and $\beta$ follow $O(1)$ holds with probability at least $1 - \delta/6$, by using the union bound, it follows that with probability at least $1 - \delta$,

$$L_D(f_{\mathbf{W}(k),a}) = \mathbb{E}_{(x,y)\sim D} \left[ \frac{1}{2} |y - f_{\mathbf{W}(k),a}(x)|^2 \right]$$

\[= (a) O \left( \frac{1}{n} \right) + O \left( \alpha R_S(\mathcal{F}_{\mathcal{R}, B}) \right) + O \left( \beta \sqrt{\frac{\log \left( \frac{n}{\lambda_0^4 \delta} \right)}{2n}} \right) \]

\[= (b) O \left( \frac{1}{n} \right) + O \left( \mathcal{R}_S(\mathcal{F}_{\mathcal{R}, B}) \right) + O \left( \sqrt{\frac{\log \left( \frac{n}{\lambda_0^4 \delta} \right)}{2n}} \right) \]

\[= (c) O \left( \sqrt{\frac{(y-u(0))^	op (H^\top)^{-1}(y-u(0))}{2n}} + \frac{\text{poly}(n, \frac{1}{\lambda_0^4 \delta})}{m^{1/4}} + \sqrt{\frac{\log \left( \frac{n}{\lambda_0^4 \delta} \right)}{2n}} \right), \quad (131) \]

where (a) follow from (130), (b) follows from the assumption that $\alpha$ and $\beta$ follow $O(1)$ for $n$, and (c) follow from (130).

Therefore, as we assume that $m = \tilde{\Omega}(\text{poly}(n, \lambda_0^{-1}, \delta^{-1}))$, we get (123) from (131).

Now we will prove the assumption that $\alpha$ and $\beta$ follow $O(1)$. From Lemma A.11, with probability at least $1 - \delta/6$, $|f_{\mathbf{W}(k),a}(x)|$ in (131) follows $O \left( \frac{\lambda_0^4 \delta}{\sqrt{\lambda_0 \delta}} \right)$ for every $k \geq 0$ and $x \sim D$. On the other hand, $y$ follows $O(1)$ for $n$. This is because $y$ is independent of $n$, as $y$ is i.i.d. sample of the model $\mathcal{D}(x, y)$. These imply that $|y - f_{\mathbf{W}(k),a}(x)|$ in (131) follows $O(1)$ for every $k \geq 0$ and $(x, y) \sim \mathcal{D}$. Therefore, $\alpha$ and $\beta$ follow $O(1)$.

\[\square\]

### A.7 Proof of Corollaries in Section 2.2

In this section, we prove Corollaries 2.3, 2.4, and 2.5, which are given sequentially as follows.

**Proof of Corollary 2.3.** Theorem 2.2 suggests that Theorem 2.1 does not hold, if $\kappa = O(n^\alpha)$ holds for some constant $\alpha < 0$ and $\lambda_0 = O(n^\beta) > 0$ holds. It is because condition $m = \Omega \left( \frac{n^6}{\lambda_0^4 \delta} \right) = \Omega(n^{6-4\gamma-2\alpha})$ in Theorem 2.1 implies condition $m = \Omega(n^{3-2\gamma})$ in Theorem 2.2 if $\kappa = O(n^\alpha)$ holds for some constant $\alpha < 0$ and $\lambda_0 = O(n) > 0$ holds.

|\[\square\]|

**Proof of Corollary 2.4.** In order for the error term $\kappa/\delta$ in (6) in Corollary 2.1 to converge to zero as $n$ increases, the condition $\kappa = o(\delta) = o(1)$ for $n$ should be satisfied. That is, $\kappa$ should follow $o(1)$ for $n$ in order for Corollary 2.1 to guarantee that the training error converges to zero. However, Corollary 2.1 does not hold under this condition of $\kappa$ if $\lambda_0 = O(n) > 0$ holds. This is because Corollary 2.3 implies that Corollary 2.1 does not hold if $\kappa = o(1)$ for $n$ holds and $\lambda_0 = O(n) > 0$ holds, as Corollary 2.1 is derived from Theorem 2.1. Therefore, if $\lambda_0 = O(n) > 0$ holds, there exists no instance of $\kappa$ satisfying both zero convergence of training error and correctness.

|\[\square\]|

**Proof of Corollary 2.5.** In order for the error term $\sqrt{\frac{\lambda_0}{\lambda_0 \delta}}$ in (7) in Corollary 2.2 to converge to zero as $n$ increases, the condition $\kappa = o(\frac{\lambda_0}{\sqrt{n}}) = o(\frac{\lambda_0}{\sqrt{\lambda_0 \delta}})$ should hold. However, Corollary 2.3 implies that Corollary 2.2 does not hold if $\kappa = o(1)$ for $n$ holds and $\lambda_0 = O(n) > 0$ holds, as Corollary 2.2 is derived from Theorem 2.1. As the condition $\kappa = o(\lambda_0/\sqrt{n})$ implies $\kappa = o(1)$ for $n$ if $\lambda_0 = O(\sqrt{n})$,
Corollary 2.2 fails to guarantee both of zero generalization error and correctness if $\lambda_0 = O(\sqrt{n})$ holds.

A.8 Experiment Details: Figure 1

All experiments are executed under the Tensorflow environment with NVIDIA Titan RTX GPU. Note that $\lambda_0$ denotes the minimum eigenvalue of $H^*$, where $X = (x_1, \ldots, x_n) \in \mathbb{R}^{d \times n}$ is set of $n$ input training samples. To plot Figure 1, we randomly select the same number of training samples for each class from 10 categories. We repeat this task 500 times; we showed the average value of $\lambda_0$ as the blue line, and shaded around this line by using the minimum/maximum values as borders.

B Proofs of Section 3

B.1 Preliminaries: Review for the existing result (Corollary 3.1) given by [2]

Before we introduce how to prove Theorems 3.2 and 3.3, we show how the existing result (Corollary 3.1) proposed by [2] was derived. We note that Corollary 3.1 proposed by [2] is a result obtained from the following Theorem B.1 (Theorem 3.1), which is Lemma F.9 in [2] (we omit to show the statement $\|W^{(h)}(t) - W^{(h)}(0)\| \leq w\sqrt{m}$ in Lemma F.9 in [2] as it does not affect in this paper).

**Theorem B.1** [Theorem 3.1, Lemma F.9 in [2]]. Suppose $m \geq \text{poly}(1/\epsilon, 1/\kappa, L, 1/\lambda_0, n, \log(1/\delta))$, where $w \leq \text{poly}(1/n, \lambda_0, 1/L, 1/\log(m), \epsilon, 1/\log(1/\delta), \kappa)$. Then with probability at least $1 - \delta$ over random initialization, we have for all $t \geq 0$

$$\|u^\kappa(t) - y\| \leq \exp\left(-\frac{1}{2}\kappa^2\lambda_0^2 t\right) \|u^\kappa(0) - y\|.$$  \hspace{0.5cm} (132)

By using Theorem B.1, Corollary 3.1 is derived as follows.

**Corollary B.1** [Corollary 3.1, Theorem 3.2 in [2]]. Let the following three conditions (a), (b), and (c) hold.

(a) $m \geq \text{poly}(1/\epsilon, 1/\kappa, L, 1/\lambda_0, n, \log(1/\delta))$

(b) $H^*$ is positive definite where $[H^*]_{i,j} = \Psi^{(L)}(x_i, x_j)$ for $i, j \in \{n\}^2$

(c) $1/\kappa = \text{poly}(1/\epsilon, \log(n/\delta))$ holds for some small constants $\epsilon, \delta > 0$.

Then, for any $x_{te} \in \mathbb{R}^d$ with $\|x_{te}\| = 1$, with probability at least $1 - \delta$ over the random initialization, we have

$$|f^\kappa(x_{te}) - f^{ntk}(x_{te})| = O(\epsilon).$$  \hspace{0.5cm} (133)

B.2 Proof of Theorem 3.2

In this section, we disprove Theorem B.1 (hence Corollary B.1). As Corollary B.1 is a corollary of Theorem B.1, it suffice to show Theorem B.1 is incorrect. We show this result in Theorem B.2 (i.e., Theorem 3.2). Before we prove Theorem B.2, we introduce the following lemmas.

We introduce the following lemma (i.e., Lemma B.1) proved by [2].
Lemma B.1 [Lemma F.7 in [2]]. Fix \( h \in \{L + 1\} \) and a sufficiently small \( w \leq \text{poly}(1/n, \lambda_0, 1/L, 1/\log(m), \epsilon, 1/\log(1/\delta), \kappa) \). Suppose for all \( t \geq 0 \), \( \|u^k(t) - y\| \leq \exp(-\frac{1}{2} \kappa^2 \lambda_0^2 t) \|u^k(0) - y\| \) and \( \|W^{(h')}(t) - W^{(h')}(0)\| \leq w\sqrt{m} \) for \( h' \neq h \). Then if \( m \geq \text{poly}(1/w) \) we have with probability at least \( 1 - \delta \) over random initialization, for all \( t \geq 0 \)

\[
\|W^{(h)}(t) - W^{(h)}(0)\| = O\left(\frac{\sqrt{n}}{\lambda_0}\right). \tag{134}
\]

We denote \( x^{(h)} \) whose \( \theta \) is given as \( \theta(t) \) by \( x^{(h)}(t) \) for \( h \in \{0 : L\} \) in (13). Then, we obtain \( x^{(h)}(t) \) is given as a constant w.r.t. \( n \) as follows.

Lemma B.2. Suppose that for every \( h \in \{L\} \), \( \|W^{(h)}(t) - W^{(h)}(0)\| \leq w\sqrt{m} \) for some constant \( w > 0 \) invariant of \( n \). Then, with probability at least \( 1 - \delta \) over random initialization, for every \( h \in \{L\} \), and for any \( x^0 \in \mathbb{R}^d \) satisfying \( \|x^0\| = 1 \), we have \( \|x^{(L)}(t)\| = O(1) \) for \( n \).

Proof of Lemma B.2. It follows that for every \( h \in \{L\} \),

\[
\|x^{(h)}(t)\| = \sqrt{\frac{c_\sigma}{m}} \|\sigma(W^{(h)}(t)x^{(h-1)}(t))\|
\]

\[
\leq \sqrt{\frac{c_\sigma}{m}} \|W^{(h)}(t)x^{(h-1)}(t)\|
\]

\[
= \sqrt{\frac{c_\sigma}{m}} \|(W^{(h)}(t) - W^{(h)}(0) + W^{(h)}(0))x^{(h-1)}(t)\|
\]

\[
= \sqrt{\frac{c_\sigma}{m}} \|(W^{(h)}(t) - W^{(h)}(0))x^{(h-1)}(t)\| + \sqrt{\frac{c_\sigma}{m}} \|W^{(h)}(0)x^{(h-1)}(t)\|
\]

\[
\leq \sqrt{\frac{c_\sigma}{m}} \|(W^{(h)}(t) - W^{(h)}(0))\| \|x^{(h-1)}(t)\| + \sqrt{\frac{c_\sigma}{m}} \|W^{(h)}(0)x^{(h-1)}(t)\|
\]

\[
\leq w\sqrt{c_\sigma} \|x^{(h-1)}(t)\| + \sqrt{\frac{c_\sigma}{m}} \|W^{(h)}(0)x^{(h-1)}(t)\|. \tag{135}
\]

From the rotational invariance of Gaussian vector, we have

\[
E_{W^{(h)}(0)} \left[ \|W^{(h)}(0)x^{(h-1)}(t)\|^2 \right] = E_{v \sim N(0,mI)} \left[ \|x^{(h-1)}(t)\|^2 \|v\|^2 \right] = m \|x^{(h-1)}(t)\|^2. \tag{136}
\]

Thus, it follows from from Markov’s inequality that \( \|W^{(h)}(0)x^{(h-1)}(t)\| \leq \sqrt{\frac{m}{p}} \|x^{(h-1)}(t)\| \) holds with a probability at least \( 1 - \delta \). By applying (136) to (135), we obtain

\[
\|x^{(h)}(t)\| \leq w\sqrt{c_\sigma} \|x^{(h-1)}(t)\| + \sqrt{\frac{c_\sigma}{\delta}} \|x^{(h-1)}(t)\|. \tag{137}
\]

Note (137) implies if \( \|x^{(h-1)}(t)\| \) follows \( O(1) \) for \( n \), then \( \|x^{(h)}(t)\| \) also follows \( O(1) \) for \( n \). As \( \|x^{(0)}(t)\| = \|x^0\| = 1 \), it follows by using the induction hypothesis and applying the union bound that with a probability at least \( 1 - \delta \),

\[
\|x^{(L)}(t)\| = O(1) \text{ for } n. \tag{138}
\]

\[\square\]
By using Lemma B.2, we also obtain an upper bound of trained network output as follows.

**Lemma B.3.** Suppose that for all \( t \geq 0 \), \( \| W^{(h')} (t) - W^{(h')} (0) \| \leq w \sqrt{m} \) for \( h' \in \{ L \} \) and \( \| u^\kappa (t) - y \| \leq \exp (- \frac{1}{2} \kappa^2 \lambda_0^2 t) \| u^\kappa (0) - y \| . \) Suppose that \( m \geq \text{poly}(1/w) \) for a sufficiently small \( w \leq \text{poly}(1/n, \lambda_0, 1/L, 1/\log(m), \epsilon, 1/\log(1/\delta), \kappa) \). Then, we have with probability at least \( 1 - \delta \) over random initialization, for all \( t \geq 0 \) and any \( x \in \mathbb{R}^d \) satisfying \( \| x \| = 1 \),

\[
\left\| f_{\theta(t)}^\kappa (x) \right\| = O \left( \frac{\kappa \sqrt{m}}{\lambda_0} \right).
\]  

**Proof of Lemma B.3.** We first prove (139) holds. From the rotational invariance of Gaussian vector, we have

\[
\mathbb{E}_{W^{(L+1)}(0)} \left[ \left\| W^{(L+1)}(0) x^{(L)}(t) \right\|^2 \right] = \mathbb{E}_{v \sim \mathcal{N}(0,1)} \left[ \left\| x^{(L)}(t) \right\|^2 v^2 \right] = \left\| x^{(L)}(t) \right\|^2.
\]

Thus, it follows from Markov's inequality that the following holds with a probability at least \( 1 - \delta \)

\[
\left\| W^{(L+1)}(0) x^{(L)}(t) \right\| \leq \sqrt{\frac{1}{\delta} \left\| x^{(L)}(t) \right\|}.
\]  

(141)

Using this fact, we have the following inequalities hold with a probability at least \( 1 - \delta \).

\[
\left\| f_{\theta(t)}^\kappa (x) \right\| = \kappa \left\| W^{(L+1)}(t) x^{(L)}(t) \right\|
\]

\[
= \kappa \left\| (W^{(L+1)}(t) - W^{(L+1)}(0)) x^{(L)}(t) \right\| + \kappa \left\| W^{(L+1)}(0) x^{(L)}(t) \right\|
\]

\[
\leq \kappa \left\| (W^{(L+1)}(t) - W^{(L+1)}(0)) \right\| \left\| x^{(L)}(t) \right\| + \kappa \left\| W^{(L+1)}(0) x^{(L)}(t) \right\|
\]

\[
\overset{(a)}{\leq} O \left( \frac{\kappa \sqrt{m}}{\lambda_0} \right) \left\| x^{(L)}(t) \right\| + \sqrt{\frac{\kappa^2}{\delta}} \left\| x^{(L)}(t) \right\|
\]

\[
\overset{(b)}{=} O \left( \frac{\kappa \sqrt{m}}{\lambda_0} \right),
\]

(142)

(143)

where \((a)\) follows from Lemma B.1 and (141) and \((b)\) follows from Lemma B.2. Therefore, (139) holds.

\( \square \)

By using Lemmas B.1,B.2, and B.3, now we are ready to prove Theorem 3.2. We rewrite Theorem 3.2 as Theorem B.2.

**Theorem B.2** [Theorem 3.2, disproof of Theorem B.1]. Suppose \( m \geq \text{poly}(1/w) \), where \( w \leq \text{poly}(1/n, \lambda_0, 1/L, 1/\log(m), \epsilon, 1/\log(1/\delta), \kappa) \). Suppose further \( \kappa = o\left( \frac{\lambda_0}{\sqrt{m}} \right) \). Then, with probability at least \( 1 - \delta \) over random initialization, there exists \( t \geq 0 \) satisfying

\[
\| u^\kappa (t) - y \| > \exp (- \frac{1}{2} \kappa^2 \lambda_0^2 t) \| u^\kappa (0) - y \| .
\]

**Proof of Theorem B.2.** From Lemma B.3, it follows that when \( \kappa = o\left( \frac{\lambda_0}{\sqrt{m}} \right) \) holds, for any \( x \in \mathbb{R}^d \) satisfying \( \| x \| = 1 \),

\[
\left\| f_{\theta(t)}^\kappa (x) \right\| = o(1).
\]  

(144)
On the other hand, Theorem B.1 implies with probability at least $1 - \delta$ over random initialization, we have for all $t \geq 0$ and all $h \in \{L + 1\}$,

$$\|u^k(t) - y\| \leq \exp(-\frac{1}{2}\kappa^2\lambda_0^2 t) \|u^k(0) - y\|. \tag{145}$$

(145) implies there exists a finite $t > 0$ satisfying $|f_{\theta(t)}^k(x_i) - y_i| \leq \epsilon$ for any $i \in \{n\}$, where $\epsilon$ is an arbitrary small constant invariant of $n$. This implies that there exists a finite $t > 0$ satisfying $y_i = \Theta(f_{\theta(t)}^k(x_i))$ for any $i \in \{n\}$. However, (144) implies that for any $i \in \{n\}$, $y_i \neq \Theta(f_{\theta(t)}^k(x_i))$ holds if $y_i = \Theta(1)$. This contraction implies Theorem B.1 does not hold when $\kappa = o(\frac{\lambda_0}{\sqrt{n}})$.

\[ \square \]

### B.3 Proof of Theorem 3.3

Before we prove Theorem 3.3, we introduce the following two lemmas (Lemmas B.4 and B.5) proposed by [2].

**Lemma B.4** [Theorem 3.1 in [2]]. Fix $\epsilon > 0$ and $\delta \in (0, 1)$. Suppose $\min_{h \in \{L\}} \|d_h\| \geq \text{poly}(L, 1/\epsilon) \log(L/\delta)$. Then, for any inputs $x, x' \in \mathbb{R}^{d_0}$ such that $\|x\| \leq 1$, $\|x'\| \leq 1$, with probability at least $1 - \delta$ we have

$$\left| \left\langle \frac{\partial f^i_\theta(x)}{\partial \theta}, \frac{\partial f^i_\theta(x')}{\partial \theta} \right\rangle - \Psi^L(x, x') \right| \leq (L + 1)\epsilon. \tag{146}$$

**Lemma B.5** [Lemma F.2 in [2]]. Fix $w \leq \text{poly}(1/L, 1/n, 1/\log(1/\delta), \lambda_0)$. Suppose we set $m \geq \text{poly}(1/w)$ and $\kappa \leq 1$. Then, with probability at least $1 - \delta$ over random initialization, we have for all $t \geq 0$, for any $(x, x') \in \{x_1, \ldots, x_n, x_{te}\} \times \{x_1, \ldots, x_n, x_{te}\}$

$$\left| \left\langle \frac{\partial f^i_\theta(x)}{\partial \theta}, \frac{\partial f^i_\theta(x')}{\partial \theta} \right\rangle \right|_{\theta=\theta(t)} - \left| \left\langle \frac{\partial f^i_\theta(x)}{\partial \theta}, \frac{\partial f^i_\theta(x')}{\partial \theta} \right\rangle \right|_{\theta=\theta(0)} \leq w. \tag{147}$$

Before we prove Theorem 3.3, we revise Lemma F.1 proposed by [2] as the following lemma. This lemma is our major contribution to prove Theorem 3.3.

**Lemma B.6** [Modification/revision of Lemma F.1 in [2]]. Let the following four assumptions hold.

(a) Matrix $E^*$ is positive definite such that $[E^*]_{i,j} = \Psi^L(x_i, x_j)$ for $i, j \in \{n + 1\}^2$ and $x_{n+1} := x_{te}$.

(b) Suppose $\max_{0 \leq t \leq \infty} \|H^* - H(t)\| \leq \epsilon_H$ holds for a small value $\epsilon_H$ such that $\lambda_{\min}(H(t)) \geq \frac{1}{2}\lambda_{\min}(H^*)$ holds for all $t \geq 0$, where $[H^*]_{i,j} = [E^*]_{i,j}$ and $[H(t)]_{i,j}$ denotes $\left\langle \frac{\partial f^i_\theta(x)}{\partial \theta}, \frac{\partial f^j_\theta(x)}{\partial \theta} \right\rangle$ for $i, j \in \{n\}^2$.

(c) Suppose $\max_{0 \leq t \leq \infty} \|\ker(x_{te}, X) - \ker_{ntk}(x_{te}, X)\| \leq \epsilon_{test}$ holds for a small value $\epsilon_{test}$.

(d) $\kappa = \Theta(1)$ for $n$.

---

Footnote 3: If $\epsilon_H$ is small enough, it follows that $\lambda_{\min}(H(t)) \geq \lambda_{\min}(H^*) - \|H^* - H(t)\| \geq \lambda_{\min}(H^*) - \epsilon_H \geq \lambda_{\min}(H^*)/2$ hence $\lambda_{\min}(H(t)) \geq \lambda_{\min}(H^*)/2$ holds.
Then, with probability at least \(1 - \delta\) over random initialization, we have

\[
|f^k(x_{te}) - f^{ntk}(x)| = O\left(\frac{\epsilon_{test}\sqrt{n}}{\lambda_0} + \frac{n}{\lambda_0^2}\log\left(\frac{n}{\epsilon_H\lambda_0\kappa}\right)\epsilon_H\right).
\]  

(148)

**Proof of Lemma B.6.** It follows that with a probability at least \(1 - \delta\),

\[
\|f^k(0)(x)\| = \kappa \|W^{(L+1)}(0)x^{(L)}(0)\| \overset{(a)}{\leq} \sqrt{\frac{\kappa^2}{\delta}} \|x^{(L)}(0)\| = O(1),
\]

where (a) follows from (141) and (b) follows from Lemma B.2. Then, from (149), it follows that

\[
\|u_k(0)\| = O(\sqrt{n}).
\]

(150)

Then, as \(\|u_k(0)\| = O(\sqrt{n})\) implies, \(\|u_k(0) - y\| = O(\sqrt{n})\) also holds. Using these facts, now we prove Lemma B.6. Our proof is based on Lemma F.1 in [2].

Let \(E^* \in \mathbb{R}^{n+1 \times n+1}\) be the Gram matrix whose \(i, j\)-th element is given as \(\Psi^L(x_i, x_j)\) with \(x_{n+1} := x_{te}\) for \(i, j \in \{n+1\}^2\). Then, \([E^*]_{i,j}\) is equal to \([H^*]_{i,j}\) for \(i, j \in \{n\}^2\). As \(E^*\) is positive definite, we can compute an eigenvector decomposition of \(E^*\) as

\[
E^* = U^\top \Pi U,
\]

(151)

where \(\Pi = \text{diag}(\pi_1, ..., \pi_{n+1})\) denotes a diagonal matrix with positive diagonal entries \((\pi_i)\) is the \(i\)-th eigenvalue of \(E^*\) and is greater than 0 as the condition (a) implies) and \(U \in \mathbb{R}^{n+1 \times n+1}\) is a unitary matrix. From (151), the \(ij\)-th element of \(E^*\) is expressed by a dot product between the following two vectors:

\[
[E^*]_{i,j} = (\Pi^{1/2}U_{i,:})^\top (\Pi^{1/2}U_{j,:})
\]

(152)

We define \(\phi_i := \Pi^{1/2}U_{i,:}\). Then, the matrix \((\phi_1, ..., \phi_{n+1}) = \Pi^{1/2}U\) has the rank \(n + 1\) as \(\Pi\) and \(U\) have the rank \(n + 1\). We recall the following \(\kappa\)-scaled kernel regression predictor

\[
f^{ntk}(x_{te}) := \ker(x_{te}, X)^\top (H^*)^{-1}y.
\]

(153)

Then, the expression in (153) can be viewed as \(f^{ntk}(x_{te}) = \kappa\phi_i^\top\beta_{ntk}\), where \(\beta_{ntk}\) satisfies

\[
\beta_{ntk} = \arg\min_\beta \|\beta\|_2
\]

such that \(\kappa\phi_i^\top\beta = y_i\) for \(i \in \{n\}\).

The solution to this minimization can be rewritten as

\[
\beta_{ntk} = \arg\min_\beta L_{ntk}(\beta; \{x_i\}_{i=1}^n) = \arg\min_\beta \sum_{i=1}^n \frac{1}{2}(\kappa\phi_i^\top\beta - y_i)^2.
\]

(155)

We assume that there exists an initialization \(\beta(0)\) satisfying \(f^{ntk}_\beta(0) := \kappa\phi_i^\top\beta(0) = f^k_{\beta(0)}(x_i)\) for \(i \in \{n+1\}\). As the matrix \((\phi_1, ..., \phi_{n+1})\) has the rank \(n + 1\), there exists \(\beta(0)\) satisfying this condition.
We let $\beta(t)$ denote the parameter $\beta$ in (155) at times $t$ trained by gradient flow and we define $f_{\beta(t)}^{ntk}(x_{te}) := \kappa \phi_{n+1}^T \beta(t)$. Then, we can rewrite (153) as an integral form as follows.

$$f_{\beta(t)}^{ntk}(x_{te}) = \int_{t=0}^{\infty} \frac{df_{\beta(t)}^{ntk}(x_{te})}{dt} dt + f_{\beta(0)}^{ntk}(x_{te}) = \int_{t=0}^{\infty} \frac{df_{\beta(t)}^{ntk}(x_{te})}{dt} dt + f_{\beta(0)}^{ntk}(x_{te}),$$  

(156)

Note the time derivative $\frac{df_{\beta(t)}^{ntk}(x_{te})}{dt}$ has the following equalities.

$$\frac{df_{\beta(t)}^{ntk}(x_{te})}{dt} = \left\langle \frac{\partial f_{\beta(t)}^{ntk}(x)}{\partial \beta(t)} , \frac{d\beta(t)}{dt} \right\rangle = - \left\langle \frac{\partial f_{\beta(t)}^{ntk}(x)}{\partial \beta(t)} , \frac{\partial L_{ntk}(\beta(t); \{x_i\}_{i=1}^n)}{\partial \beta(t)} \right\rangle$$

$$= - \left\langle \frac{\partial f_{\beta(t)}^{ntk}(x_{te})}{\partial \beta(t)} , \sum_{i=1}^n (u_{ntk,i}(t) - y_i) \frac{\partial f_{\beta(t)}^{ntk}(x_i)}{\partial \beta(t)} \right\rangle$$

$$= - \left\langle \kappa \phi_{n+1}, \sum_{i=1}^n \kappa (u_{ntk,i}(t) - y_i) \phi_i \right\rangle$$

$$= -\kappa^2 \text{ker}_{ntk}(x_{te}, X)^T (u_{ntk}(t) - y),$$  

(157)

where $u_{ntk}(t) = (u_{ntk,1}(t), ..., u_{ntk,n}(t))^T \in \mathbb{R}^n$, $u_{ntk,i}(t) = f_{\beta(t)}^{ntk}(x_i)$ for $i \in \{n\}$, and $\text{ker}_{ntk}(x_{te}, X) = (\phi_{n+1}^T \phi_1, ..., \phi_{n+1}^T \phi_n)$. Similarly, for the neural network, we have

$$\frac{df_{\theta(t)}^{\kappa}(x_{te})}{dt} = \left\langle \frac{\partial f_{\theta(t)}^{\kappa}(x)}{\partial \theta(t)} , \frac{d\theta(t)}{dt} \right\rangle$$

$$= - \left\langle \frac{\partial f_{\theta(t)}^{\kappa}(x_{te})}{\partial \theta(t)} , \frac{\partial L(\theta(t))}{\partial \theta(t)} \right\rangle$$

$$= - \left\langle \frac{\partial f_{\theta(t)}^{\kappa}(x_{te})}{\partial \theta(t)} , \sum_{i=1}^n (u_{i}^\kappa(t) - y_i) \frac{\partial f_{\theta(t)}^{\kappa}(x_i)}{\partial \theta(t)} \right\rangle$$

$$= -\kappa^2 \text{ker}_i(x_{te}, X)^T (u_{i}^\kappa(t) - y),$$  

(158)

where $u_{i}^\kappa(t) = (u_{i}^\kappa(t), ..., u_{i}^\kappa(t))^T \in \mathbb{R}^n$, $u_{i}^\kappa(t) = f_{\theta(t)}^{\kappa}(x_i)$ for $i \in \{n\}$, $\text{ker}_i(x_{te}, X) = (\text{ker}_i(x_{te}, x_1), ..., \text{ker}_i(x_{te}, x_n))^T$, and $\text{ker}_i(x_{te}, x_i) = \left\langle \frac{df_{\theta(t)}^{\kappa}(x_{te})}{d\theta(t)} , \frac{df_{\theta(t)}^{\kappa}(x_i)}{d\theta(t)} \right\rangle$ for $i \in \{n\}$.

Then, the gap between the neural network and the kernel regression predictor has the following
As \( \lambda \exp(t) \)

Next, we will show the second term in (159) is bounded as follows

\[
| f^\kappa(x) - f^{ntk}(x) |
= \left| f^{\kappa}_{\beta(0)}(x) - f^{\kappa}_{\beta(0)}(x) + \int_{t=0}^{\infty} \left( \frac{df^{\kappa}_{\beta(t)}}{dt} - \frac{df^{\kappa}_{\beta(t)}}{dt} \right) dt \right|
= \left| \int_{t=0}^{\infty} \left( \frac{df^{\kappa}_{\beta(t)}}{dt} - \frac{df^{\kappa}_{\beta(t)}}{dt} \right) dt \right|
\leq -\kappa^2 \int_{t=0}^{\infty} \left( \ker(x) - \ker^{ntk}(x) \right) (u^\kappa(t) - y) dt
\leq \kappa^2 \int_{t=0}^{\infty} \left( \ker(x) - \ker^{ntk}(x) \right) (u^\kappa(t) - y) dt
\]

As \( \lambda_{\min}(H(t)) \geq \frac{1}{2} \lambda_0 \) holds for all \( t \geq 0 \) by the assumption, it follows from \( \frac{du(t)}{dt} = -\kappa^2 H(t) (u^\kappa(t) - y) \) that \( \|u^\kappa(t) - y\| \leq \exp(-\frac{\kappa^2}{2} \lambda_0 t) \|u^\kappa(0) - y\| \). Therefore, the first term in (159) is bounded as follows

\[
\kappa^2 \varepsilon_{\text{test}} \int_{t=0}^{\infty} \|u^\kappa(t) - y\| dt
= \kappa^2 \varepsilon_{\text{test}} \int_{t=0}^{\infty} \exp(-\frac{\kappa^2}{2} \lambda(t)) \|u^\kappa(0) - y\| dt
= \kappa^2 \varepsilon_{\text{test}} O\left( \frac{\varepsilon_{\text{H}}}{\sqrt{n}} \right)
= O\left( \frac{\varepsilon_{\text{H}}}{\sqrt{n}} \right).
\]  

Next, we will show the second term in (159) is bounded as follows

\[
\kappa^2 \max_{0 \leq t \leq \infty} \|\ker^{ntk}(x)\|| \int_{t=0}^{\infty} \|u^\kappa(t) - u^{ntk}(t)\| dt = O\left( \frac{n \log^2}{\lambda_0^2} \right) \varepsilon_{\text{H}}.
\]  

As \( \lambda_{\min}(H(t)) \geq \frac{1}{2} \lambda_0 \) holds for all \( t \geq 0 \) by the assumption, it follows that \( \|u^\kappa(t) - y\| \leq \exp(-\frac{\kappa^2}{2} \lambda_0 (t - t_0)) \|u^\kappa(t_0) - y\| \). And similarly, as \( \lambda_{\min}(H) \) holds, it follows from \( \frac{du^{ntk}(t)}{dt} = -\kappa^2 H^\kappa(u^{ntk}(t) - y) \) that \( \|u^{ntk}(t) - y\| \leq \exp(-\frac{\kappa^2}{2} \lambda_0 (t - t_0)) \|u^{ntk}(t_0) - y\| \). Thus,

\[
\int_{t=t_0}^{\infty} \|u^\kappa(t) - y\| dt = \int_{t=t_0}^{\infty} \exp(-\frac{\kappa^2}{2} \lambda_0 (t - t_0)) \|u^\kappa(t_0) - y\| dt = O\left( \frac{\|u^\kappa(t_0) - y\|}{\kappa^2 \lambda_0^2} \right)
\]

\[
\int_{t=t_0}^{\infty} \|u^{ntk}(t) - y\| dt = \int_{t=t_0}^{\infty} \exp(-\frac{\kappa^2}{2} \lambda_0 (t - t_0)) \|u^{ntk}(t_0) - y\| dt = O\left( \frac{\|u^{ntk}(t_0) - y\|}{\kappa^2 \lambda_0^2} \right).
\]
From (162) and (163), it follows that if \( t_0 = \frac{C}{\kappa_0 \epsilon H} \log \left( \frac{n}{\lambda_0^2} \right) \) for some \( C \),
\[
\int_{t=t_0}^{\infty} \| u^{\kappa}(t) - u_{ntk}(t) \| \ dt \leq \int_{t=t_0}^{\infty} \| u^{\kappa}(t) - y \| \ dt + \int_{t=t_0}^{\infty} \| u_{ntk}(t) - y \| \ dt
\]
\[= O \left( \frac{\| u^{\kappa}(t_0) - y \| + \| u_{ntk}(t_0) - y \|}{\kappa_0 \lambda_0} \right) \]
\[= O \left( \frac{\sqrt{n}}{\kappa_0 \lambda_0} \exp(-\lambda_0 \kappa^2 t_0) \right) \]
\[= O(\epsilon H). \]

On the other hand, we obtain
\[
\| u^{\kappa}(t) - u_{ntk}(t) \| \leq \| u^{\kappa}(0) - u_{ntk}(0) \| + \int_{\tau=0}^{t} \left\| \frac{d(u^{\kappa}(\tau) - u_{ntk}(\tau))}{d\tau} \right\| d\tau
\]
\[= \int_{\tau=0}^{t} \left\| \frac{d(u^{\kappa}(\tau) - u_{ntk}(\tau))}{d\tau} \right\| d\tau, \tag{164} \]
where the equality follows from our setting of the initialization \( \beta(0) \) implying that \( u^{\kappa}(0) = u_{ntk}(0) \).

We also note
\[
\frac{d(u^{\kappa}(\tau) - u_{ntk}(\tau))}{d\tau} = -\kappa^2 H(\tau)(u^{\kappa}(\tau) - y) + \kappa^2 H^*(u_{ntk}(\tau) - y)
\]
\[= -\kappa^2 H^*(u^{\kappa}(\tau) - u_{ntk}(\tau)) + \kappa^2 (H^* - H(\tau))(u^{\kappa}(\tau) - y). \tag{165} \]

As \( H^* \) is positive semidefinite, the first term in (165) only makes \( \| u^\kappa(t) - u_{ntk}(t) \| \) smaller. Then, from (164) and (165), we obtain
\[
\| u^{\kappa}(t) - u_{ntk}(t) \| \leq \int_{\tau=0}^{t} \left\| \frac{d(u^{\kappa}(\tau) - u_{ntk}(\tau))}{d\tau} \right\| d\tau
\]
\[\leq \int_{\tau=0}^{t} \| \kappa^2 (H^* - H(\tau))(u^{\kappa}(\tau) - y) \| d\tau
\]
\[\leq \kappa^2 \int_{\tau=0}^{t} \| H^* - H(\tau) \| \| u^{\kappa}(\tau) - y \| d\tau
\]
\[\leq t \kappa^2 \epsilon H \| u^{\kappa}(0) - y \|
\]
\[= O(t \kappa^2 \epsilon H \sqrt{n}). \]

By setting \( t = t_0 = \frac{C}{\kappa_0 \epsilon H} \log \left( \frac{n}{\lambda_0^2} \right) \), it follows that
\[
\int_{t=0}^{t_0} \| u^{\kappa}(t) - u_{ntk}(t) \| \ dt = O(t_0^2 \kappa^2 \epsilon H \sqrt{n}) = O \left( \frac{\sqrt{n}}{\lambda_0^2 \kappa_0} \log \left( \frac{n}{\epsilon H \lambda_0} \right)^2 \epsilon H \right). \tag{166} \]

By applying (166) to the second term in (159), we get
\[
\kappa^2 \max_{0 \leq t \leq \infty} \| \ker_{ntk}(x_t, X) \| \int_{t=0}^{\infty} \| u^{\kappa}(t) - u_{ntk}(t) \| \ dt = \max_{0 \leq t \leq \infty} \| \ker_{ntk}(x_t, X) \| O \left( \frac{\sqrt{n}}{\lambda_0^2} \log \left( \frac{n}{\epsilon H \lambda_0} \right)^2 \epsilon H \right). \tag{167} \]
As \( \| \ker_{ntk}(x_{te}, X) \| = \sqrt{\sum_{i \in \{n\}} (\phi_{n+1}^i)^2} = \sqrt{\sum_{i \in \{n\}} (E_{n+1,i})^2} = O(\sqrt{n}) \) where the last equality follows from the fact that each element of \( E^* \) is bounded as a constant w.r.t. \( n \) (as the \( ij \)-th value of \( E^* \) depends only \( x_i \) and \( x_j \) according to the definition of \( E^* \)), it follows from (167) that

\[
\kappa^2 \max_{0 \leq t \leq \infty} \| \ker_{ntk}(x_{te}, X) \| \int_{t=0}^{\infty} \| u^{\kappa}(t) - u_{ntk}(t) \| \, dt = O\left( \frac{n}{\lambda_0^2} \log \left( \frac{n}{\epsilon_H \lambda_0} \right)^2 \epsilon_H \right). \tag{168}
\]

Therefore, (161) holds.

By applying (160) and (161) to (159), we get

\[
|f^\kappa(x_{te}) - f^{ntk}(x_{te})| = O\left( \frac{\epsilon_{test} \sqrt{n}}{\lambda_0} + \frac{n}{\lambda_0^2} \log \left( \frac{n}{\epsilon_H \lambda_0} \right)^2 \epsilon_H \right).
\]

Now, we are ready to prove Theorem 3.3 by using Lemmas B.4, B.5, and B.6. We rewrite Theorem 3.3 as the following theorem.

**Theorem B.3** [Theorem 3.3, modification/revision of Theorem 3.2 in [2]]. For any \( \epsilon > 0 \) and any \( x_{te} \in \mathbb{R}^d \) with \( \| x_{te} \| = 1 \), let the following three conditions \( (a), (b), \) and \( (c) \) hold.

\( (a) \) \( m \geq \text{poly}(1/\epsilon, 1/\kappa, L, 1/\lambda_0, n, \log(1/\delta)) \)

\( (b) \) Matrix \( E^* \) is positive definite such that \( [E^*]_{i,j} = \Psi(L)(x_i, x_j) \) for \( i, j \in \{n+1\}^2 \) and \( x_{n+1} := x_{te} \).

\( (c) \) \( \kappa = 1 \)

Then, with probability at least 1 – \( \delta \) over the random initialization, we have

\[
|f^\kappa(x_{te}) - f^{ntk}(x_{te})| = O(\epsilon).
\]

**Proof of Theorem B.3.** Our proof is based on Theorem 3.2 in [2]. Lemma B.4 implies there exists a small value \( \epsilon_H \) satisfying \( \frac{n}{\lambda_0^2} \log \left( \frac{n}{\epsilon_H \lambda_0} \right)^2 \epsilon_H \leq \epsilon \) and the following condition at the same time, if the network width \( m \) is sufficiently large as the condition \( (a) \) holds for an arbitrarily small value \( \epsilon > 0 \).

- Suppose \( \max_{0 \leq t \leq \infty} \| H^* - H(t) \| \leq \epsilon_H \) holds for a small value \( \epsilon_H \) such that \( \lambda_{\min}(H(t)) \geq \frac{1}{2} \lambda_{\min}(H^*) \) holds for all \( t \geq 0 \), where \( [H^*]_{i,j} = [E^*]_{i,j} \) for \( i, j \in \{n\}^2 \).

Lemma B.5 implies there exists a small value \( \epsilon_{test} \) satisfying \( \frac{\epsilon_{test} \sqrt{n}}{\lambda_0} \leq \epsilon \) and the following condition at the same time, if the network width \( m \) is sufficiently large as the condition \( (a) \) holds for an arbitrarily small value \( \epsilon > 0 \).

- Suppose \( \max_{0 \leq t \leq \infty} \| \ker_t(x_{te}, X) - \ker_{ntk}(x_{te}, X) \| \leq \epsilon_{test} \) holds for a small value \( \epsilon_{test} \).

Therefore, we complete the proof by applying the above two results to (148) in Lemma B.6. \( \square \)
B.4 Proof of Corollary 3.2

In this section, we prove Corollary 3.2, which is given as follows.

Proof of Corollary 3.2. From the assumption $\lambda_0 = O(1)$ for $n$, $\kappa = o(\frac{\lambda_0}{\sqrt{n}})$ in Theorem 3.2 implies $\kappa = o(\frac{1}{\sqrt{n}})$. And $\kappa = \text{poly}(1/n)$ implies $\kappa = o(\frac{1}{\sqrt{n}})$. Therefore, we have the fact that $\kappa = \text{poly}(1/n)$ implies $\kappa = o(\frac{\lambda_0}{\sqrt{n}})$ in Theorem 3.2.

On the other hand, in order for Corollary 3.1 to guarantee the gap $\epsilon$ between trained network and NKRP converges to zero as $n$ increases (i.e., $\epsilon = O(n^\alpha)$ for some $\alpha < 0$), from the condition of $\kappa = 1/\text{poly}(1/\epsilon)$, $\kappa$ should decrease w.r.t. $n$ as a polynomial function with input $1/n$ as follows

$$\kappa = 1/\text{poly}(1/\epsilon) = 1/\text{poly}(n^{-\alpha}) = \text{poly}(n^\alpha) = \text{poly}(1/n).$$

(169)

However, under the condition $\kappa = \text{poly}(1/n)$ in (169), it follows from Theorem 3.2 that Theorem 3.1 (hence Corollary 3.1) does not hold as $\kappa = \text{poly}(1/n)$ implies $\kappa = o(\frac{\lambda_0}{\sqrt{n}})$ in Theorem 3.2.

Therefore, Corollary 3.1 fails to guarantee $\epsilon$ in (20) converges to zero as $n$ increases. 

\[\square\]