Fine-Grained Analysis of Optimization and Generalization for Overparameterized Two-Layer Neural Networks

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Abstract

Recent works have cast some light on the mystery of why deep nets fit any data and generalize despite being very overparametrized. This paper analyzes training and generalization for a simple 2-layer ReLU net with random initialization, and provides the following improvements over recent works:

(i) Using a tighter characterization of training speed than recent papers, an explanation for why training a neural net with random labels leads to slower training, as originally observed in [Zhang et al. ICLR'17].

(ii) Generalization bound independent of network size, using a data-dependent complexity measure. Our measure distinguishes clearly between random labels and true labels on MNIST and CIFAR, as shown by experiments. Moreover, recent papers require sample complexity to increase (slowly) with the size, while our sample complexity is completely independent of the network size.

(iii) Learnability of a broad class of smooth functions by 2-layer ReLU nets trained via gradient descent.

The key idea is to track dynamics of training and generalization via properties of a related kernel.

1. Introduction

The well-known work of Zhang et al. (2017) highlighted intriguing experimental phenomena about deep net training – specifically, optimization and generalization – and asked whether theory could explain them. They showed that sufficiently powerful nets (with vastly more parameters than number of training samples) can attain zero training error, regardless of whether the data is properly labeled or randomly labeled. Obviously, training with randomly labeled data cannot generalize, whereas training with properly labeled data generalizes. See Figure 2 replicating some of these results.

Recent papers have begun to provide explanations, showing that gradient descent can allow an overparametrized multi-layer net to attain arbitrarily low training error on fairly generic datasets (Du et al., 2018a;c; Li & Liang, 2018; Allen-Zhu et al., 2018b; Zou et al., 2018), provided the amount of overparametrization is a high polynomial of the relevant parameters (i.e. vastly more than the overparametrization in (Zhang et al., 2017)). Under further assumptions it can also be shown that the trained net generalizes (Allen-Zhu et al., 2018a). But some issues were not addressed in these papers, and the goal of the current paper is to address them.

First, the experiments in (Zhang et al., 2017) show that though the nets attain zero training error on even random data, the convergence rate is much slower. See Figure 1.

Question 1. *Why do true labels give faster convergence rate than random labels for gradient descent?*

The above papers do not answer this question, since their proof of convergence does not distinguish between good and random labels.

The next issue is about generalization: clearly, some property of properly labeled data controls generalization, but what? Classical measures used in generalization theory such as VC-dimension and Rademacher complexity are much too pessimistic. A line of research proposed norm-based (e.g. (Bartlett et al., 2017a)) and compression-based bounds (Arora et al., 2018). But the sample complexity upper bounds obtained are still far too weak. Furthermore they rely on some property of the trained net that is *revealed/computed* at the end of training. There is no property of data alone that determine upfront whether the trained net will generalize. A recent paper (Allen-Zhu et al., 2018a) assumed that there exists an underlying (unknown) neural network that achieves low error on the data distribution, and the amount of data available is quite a bit more than the min-

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imum number of samples needed to learn this underlying neural net. Under this condition, the overparametrized net (which has way more parameters) can learn in a way that generalizes. However, it is hard to verify from data whether this assumption is satisfied, even after the larger net has finished training.[1] Thus the assumption is in some sense unverifiable.

Question 2. *Is there an easily verifiable complexity measure that can differentiate true labels and random labels?*

Without explicit regularization, to attack this problem, one must resort to algorithm-dependent generalization analysis. One such line of work established that first-order methods can automatically find minimum-norm/maximum-margin solutions that fit the data in the settings of logistic regression, deep linear networks, and symmetric matrix factorization (Soudry et al., 2018; Gunasekar et al., 2018a;b; Ji & Telgarsky, 2018; Li et al., 2018b). However, how to extend these results to non-linear neural networks remains unclear (Wei et al., 2018). Another line of algorithm-dependent analysis of generalization (Hardt et al., 2015; Mou et al., 2017; Chen et al., 2018) used stability of specific optimization algorithms that satisfy certain generic properties like convexity, smoothness, etc. However, as the number of epochs becomes large, these generalization bounds are vacuous.

Our results. We give a new analysis that provides answers to Questions 1 and 2 for overparameterized two-layer neural networks with ReLU activation trained by gradient descent (GD), when the number of neurons in the hidden layer is sufficiently large. In this setting, Du et al. (2018c) have proved that GD with random initialization can achieve zero training error for any non-degenerate data. We give a more refined analysis of the trajectory of GD which enables us to provide answers to Questions 1 and 2. In particular:

- In Section 4, using the trajectory of the network predictions on the training data during optimization, we accurately estimate the magnitude of training loss in each iteration. Our key finding is that the number of iterations needed to achieve a target accuracy depends on the projections of data labels on the eigenvectors of a certain Gram matrix to be defined in Equation (3). On MNIST and CIFAR datasets, we find that such projections are significantly different for true labels and random labels, and as a result we are able to answer Question 1.
- In Section 5, we give a generalization bound for the solution found by GD, based on accurate estimates of how much the network parameters can move during optimization (in suitable norms). Our generalization bound depends on a *data-dependent complexity measure* (c.f. Equation (10)), and notably, is completely independent of the number of hidden units in the network. Again, we test this complexity measure on MNIST and CIFAR, and find that the complexity measures for true and random labels are significantly different, which thus answers Question 2.

  Notice that because zero training error is achieved by the solution found by GD, a generalization bound is an upper bound on the error on the data distribution (test error). We also remark that our generalization bound is valid for *any data labels* – it does not require the existence of a small ground-truth network as in (Allen-Zhu et al., 2018a). Moreover, our bound can be efficiently computed for any data labels.
- In Section 6, we further study what kind of functions can be provably learned by two-layer ReLU networks trained by GD. Combining the optimization and generalization results, we uncover a broad class of learnable functions, including linear functions, two-layer neural networks with polynomial activation $\phi(z) = z^{2l}$ or cosine activation, etc. Our requirement on the smoothness of learnable functions is weaker than that in (Allen-Zhu et al., 2018a).

Finally, we note that the intriguing generalization phenomena in deep learning were observed in kernel methods as well (Belkin et al., 2018). The analysis in the current paper is also related to a kernel from the ReLU activation (c.f. Equation (3)).

2. Related Work

In this section we survey previous works on optimization and generalization aspects of neural networks.

Optimization. Many papers tried to characterize geometric landscapes of objective functions (Safran & Shamir, 2017; Zhou & Liang, 2017; Freeman & Bruna, 2016; Hardt & Ma, 2016; Nguyen & Hein, 2017; Kawaguchi, 2016; Venturi et al., 2018; Soudry & Carmon, 2016; Du & Lee, 2018; Soltanolkotabi et al., 2018; Haeffele & Vidal, 2015). The hope is to leverage recent advance in first-order algorithms (Ge et al., 2015; Lee et al., 2016; Jin et al., 2017) which showed that if the landscape satisfies (1) all local minima are global and (2) all saddle points are strict (i.e., there exists a negative curvature), then first-order methods can escape all saddle points and find a global minimum. Unfortunately, these desired properties do not hold even for simple non-linear shallow neural networks (Yun et al., 2018) or 3-layer linear neural networks (Kawaguchi, 2016).

Another approach is to directly analyze trajectory of the optimization method and to show convergence to global mini-

[1] In Section 2, we discuss the related works in more details.

mum. A series of papers made strong assumptions on input distribution as well as realizability of labels, and showed global convergence of (stochastic) gradient descent for some shallow neural networks (Tian, 2017; Soltanolkotabi, 2017; Brutzkus & Globerson, 2017; Du et al., 2017a;b; Li & Yuan, 2017). Some local convergence results have also been proved (Zhong et al., 2017; Zhang et al., 2018). However, these assumptions are not satisfied in practice.

For two-layer neural networks, a line of papers used mean field analysis to establish that for infinitely wide neural networks, the empirical distribution of the neural network parameters can be described as a Wasserstein gradient flow (Mei et al., 2018; Chizat & Bach, 2018a; Sirignano & Spiliopoulos, 2018; Rotskoff & Vanden-Eijnden, 2018; Wei et al., 2018). However, it is unclear whether this framework can explain the behavior of first-order methods on finite-size neural networks.

Recent breakthroughs were made in understanding optimization of overparameterized neural networks through the trajectory-based approach. They proved global polynomial time convergence of (stochastic) gradient descent on non-linear neural networks for minimizing empirical risk. Their proof techniques can be roughly classified into two categories. Li & Liang (2018); Allen-Zhu et al. (2018b); Zou et al. (2018) analyzed the trajectory of parameters and showed that on the trajectory, the objective function satisfies certain gradient dominance property. On the other hand, (Du et al., 2018a;c) analyzed the trajectory of network predictions on training samples and showed that it enjoys a strongly-convex-like property.

Generalization. It is well known that the VC-dimension of neural networks is at least linear in the number of parameters (Bartlett et al., 2017b), and therefore classical VC theory cannot explain the generalization ability of modern neural networks with more parameters than training samples. Researchers have proposed norm-based generalization bounds (Bartlett & Mendelson, 2002; Bartlett et al., 2017a; Neyshabur et al., 2015; 2017; 2019; Konstantinos et al., 2017; Golowich et al., 2017; Li et al., 2018a) and compression-based bounds (Arora et al., 2018). Dziugaite & Roy (2017); Zhou et al. (2019) used the PAC-Bayes approach to compute non-vacuous generalization bounds for MNIST and ImageNet, respectively. All these bounds are *posterior* in nature – they depend on certain properties of the *trained* neural networks. Therefore, one has to finish training a neural network to know whether it can generalize. Comparing with these results, our generalization bound only depends on training data and can be calculated without actually training the neural network.

Another line of work assumed the existence of a true model, and showed that the (regularized) empirical risk minimizer has good generalization with sample complexity that depends on the true model (Du et al., 2018b; Ma et al., 2018; Imaizumi & Fukumizu, 2018). These papers ignored the difficulty of optimization, while we are able to prove generalization of the solution found by gradient descent. Furthermore, our generic generalization bound does not assume the existence of any true model.

Our paper is closely related to (Allen-Zhu et al., 2018a) which showed that two-layer overparametrized neural networks trained by randomly initialized stochastic gradient descent can learn a class of infinite-order smooth functions. In contrast, our generalization bound depends on a data-dependent complexity measure that can be computed for any dataset, without assuming any ground-truth model. Furthermore, as a consequence of our generic bound, we also show that two-layer neural networks can learn a class of infinite-order smooth functions, with a less strict requirement for smoothness. Allen-Zhu et al. (2018a) also studied the generalization performance of three-layer neural nets.

Lastly, our work is related to kernel methods, especially recent discoveries of the connection between deep learning and kernels (Jacot et al., 2018; Chizat & Bach, 2018b; Daniely et al., 2016; Daniely, 2017). Our analysis utilized several properties of a related kernel from the ReLU activation (c.f. Equation (3)).

3. Preliminaries and Overview of Results

Notation. We use bold-faced letters for vectors and matrices. For a matrix $\mathbf{A}$, let $\mathbf{A}_{ij}$ be its (i,j)-th entry. We use $\|\cdot\|_2$ to denote the Euclidean norm of a vector or the spectral norm of a matrix, and use $\|\cdot\|_F$ to denote the Frobenius norm of a matrix. Denote by $\lambda_{\min}(\mathbf{A})$ the minimum eigenvalue of a symmetric matrix $\mathbf{A}$. Let $\mathrm{vec}\left(\mathbf{A}\right)$ be the vectorization of a matrix $\mathbf{A}$ in column-first order. Let $\mathbf{I}$ be the identity matrix and $[n] = \{1, 2, \ldots, n\}$. Denote by $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ the Gaussian distribution with mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$. Denote by $\sigma\left(\cdot\right)$ the ReLU function $\sigma\left(z\right) = \max\{z, 0\}$. Denote by $\mathbb{I}\{E\}$ the indicator function for an event E.

3.1. Setting: Two-Layer Neural Network Trained by Randomly Initialized Gradient Descent

We consider a two-layer ReLU activated neural network with m neurons in the hidden layer:

$$f_{\mathbf{W},\mathbf{a}}(\mathbf{x}) = \frac{1}{\sqrt{m}} \sum_{r=1}^{m} a_r \sigma\left(\mathbf{w}_r^\top \mathbf{x}\right),$$

where $\mathbf{x} \in \mathbb{R}^d$ is the input, $\mathbf{w}_1, \ldots, \mathbf{w}_m \in \mathbb{R}^d$ are weight vectors in the first layer, $a_1, \ldots, a_m \in \mathbb{R}$ are weights in the second layer. For convenience we denote $\mathbf{W} = (\mathbf{w}_1, \ldots, \mathbf{w}_m) \in \mathbb{R}^{d \times m}$ and $\mathbf{a} = (a_1, \ldots, a_m)^\top \in \mathbb{R}^m$.

We are given n input-label samples $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ drawn i.i.d. from an underlying data distribution $\mathcal{D}$ over $\mathbb{R}^d \times \mathbb{R}$. We denote $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n) \in \mathbb{R}^{d \times n}$ and $\mathbf{y} = (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$. For simplicity, we assume that for $(\mathbf{x}, y)$ sampled from $\mathcal{D}$, we have $\|\mathbf{x}\|_2 = 1$ and $|y| \le 1$.

We train the neural network by *randomly initialized gradient descent (GD)* on the quadratic loss over data S. In particular, we first initialize the parameters randomly:

$$\mathbf{w}_r(0) \sim \mathcal{N}(\mathbf{0}, \kappa^2 \mathbf{I}), a_r \sim \text{unif}\left(\{-1, 1\}\right), \quad \forall r \in [m], \tag{1}$$

where $0 < \kappa \le 1$ controls the magnitude of initialization, and all randomnesses are independent. We then fix the second layer $\mathbf{a}$ and optimize the first layer $\mathbf{W}$ through GD on the following objective function:

$$\Phi(\mathbf{W}) = \frac{1}{2} \sum_{i=1}^n \left(y_i - f_{\mathbf{W},\mathbf{a}}(\mathbf{x}_i)\right)^2. \tag{2}$$

The GD update rule can be written as:[2]

$$\begin{aligned} \mathbf{w}_r(k+1) - \mathbf{w}_r(k) &= -\eta \frac{\partial \Phi(\mathbf{W}(k))}{\partial \mathbf{w}_r} \\ = -\eta \frac{a_r}{\sqrt{m}} &\sum_{i=1}^n (f_{\mathbf{W}(k),\mathbf{a}}(\mathbf{x}_i) - y_i) \mathbb{I}\left\{\mathbf{w}_r(k)^\top \mathbf{x}_i \ge 0\right\} \mathbf{x}_i, \end{aligned}$$

where $\eta > 0$ is the learning rate.

3.2. The Gram Matrix from ReLU Kernel

Given $\{\mathbf{x}_i\}_{i=1}^n$, we define the following *Gram matrix* $\mathbf{H}^\infty \in \mathbb{R}^{n \times n}$ as follows:

$$\begin{aligned} \mathbf{H}^\infty_{ij} &= \mathbb{E}_{\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[\mathbf{x}_i^\top \mathbf{x}_j \mathbb{I}\left\{\mathbf{w}^\top \mathbf{x}_i \ge 0, \mathbf{w}^\top \mathbf{x}_j \ge 0\right\}\right] \\ &= \frac{\mathbf{x}_i^\top \mathbf{x}_j \left(\pi - \arccos(\mathbf{x}_i^\top \mathbf{x}_j)\right)}{2\pi}, \quad \forall i, j \in [n]. \end{aligned} \tag{3}$$

This matrix can be viewed as a Gram matrix from a kernel associated with the ReLU function, and has been studied in (Xie et al., 2017; Tsuchida et al., 2017; Du et al., 2018c).

In our setting of training a two-layer ReLU network, Du et al. (2018c) showed that if $\mathbf{H}^\infty$ is positive definite, GD converges to 0 training loss if m is sufficiently large:

Theorem 3.1 ((Du et al., 2018c)[3]). *Assume $\lambda_0 = \lambda_{\min}(\mathbf{H}^\infty) > 0$. For $\delta \in (0, 1)$, if $m = \Omega\left(\frac{n^6}{\lambda_0^4 \kappa^2 \delta^3}\right)$ and $\eta = O\left(\frac{\lambda_0}{n^2}\right)$, then with probability at least $1 - \delta$ over the random initialization* (1)*, we have:*

- $\Phi(\mathbf{W}(0)) = O(n/\delta)$;
- $\Phi(\mathbf{W}(k+1)) \le \left(1 - \frac{\eta \lambda_0}{2}\right) \Phi(\mathbf{W}(k)), \ \forall k \ge 0.$

Our results on optimization and generalization also crucially depend on this matrix $\mathbf{H}^\infty$.

3.3. Overview of Our Results

Now we give an informal description of our main results. It assumes that the initialization magnitude κ is sufficiently small and the network width m is sufficiently large (to be quantified later).

The following theorem gives a precise characterization of how the objective decreases to 0. It says that this process is essentially determined by a power method for matrix $\mathbf{I} - \eta \mathbf{H}^\infty$ applied on the label vector $\mathbf{y}$.

Theorem 3.2 (Informal version of Theorem 4.1)**.** *With high probability we have:*

$$\Phi(\mathbf{W}(k)) \approx \frac{1}{2} \left\|(\mathbf{I} - \eta \mathbf{H}^\infty)^k \mathbf{y}\right\|_2^2, \quad \forall k \ge 0.$$

As a consequence, we are able to distinguish the convergence rates for different labels $\mathbf{y}$, which can be determined by the projections of $\mathbf{y}$ on the eigenvectors of $\mathbf{H}^\infty$. This allows us to obtain an answer to Question 1. See Section 4 for details.

Our main result for generalization is the following:

Theorem 3.3 (Informal version of Theorem 5.1)**.** *For any 1-Lipschitz loss function, the generalization error of the two-layer ReLU network found by GD is at most*

$$\sqrt{\frac{2\mathbf{y}^\top (\mathbf{H}^\infty)^{-1} \mathbf{y}}{n}}. \tag{4}$$

Notice that our generalization bound (4) can be computed from data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, and is completely independent of the network width m. We observe that this bound can clearly distinguish true labels and random labels, thus providing an answer to Question 2. See Section 5 for details.

Finally, using Theorem 3.3, we prove that we can use our two-layer ReLU network trained by GD to learn a broad class of functions, including linear functions, two-layer neural networks with polynomial activation $\phi(z) = z^{2l}$ or cosine activation, etc. See Section 6 for details.

3.4. Additional Notation

We introduce some additional notation that will be used.

Define $u_i = f_{\mathbf{W},\mathbf{a}}(\mathbf{x}_i)$, i.e., the network's prediction on the i-th input. We also use $\mathbf{u} = (u_1, \ldots, u_n)^\top \in \mathbb{R}^n$ to denote all n predictions. Then we have $\Phi(\mathbf{W}) = \frac{1}{2}\|\mathbf{y} - \mathbf{u}\|_2^2$ and

[2] Since ReLU is not differentiable at 0, we just define "gradient" using this formula, and this is indeed what is used in practice.

[3] Du et al. (2018c) only considered the case $\kappa = 1$, but it is straightforward to generalize their result to general κ at the price of an extra $1/\kappa^2$ factor in m.

the gradient of Φ can be written as:

$$\frac{\partial \Phi(\mathbf{W})}{\partial \mathbf{w}_r} = \frac{1}{\sqrt{m}} a_r \sum_{i=1}^{n} (u_i - y_i) \mathbb{I}_{r,i} \mathbf{x}_i, \quad \forall r \in [m], \quad (5)$$

where $\mathbb{I}_{r,i} = \mathbb{I}\left\{\mathbf{w}_r^\top \mathbf{x}_i \geq 0\right\}$.

We define two matrices $\mathbf{Z}$ and $\mathbf{H}$ which will play a key role in our analysis of the GD trajectory:

$$\mathbf{Z} = \frac{1}{\sqrt{m}} \begin{pmatrix} \mathbb{I}_{1,1} a_1 \mathbf{x}_1 & \cdots & \mathbb{I}_{1,n} a_1 \mathbf{x}_n \\ \vdots & \ddots & \vdots \\ \mathbb{I}_{m,1} a_m \mathbf{x}_1 & \cdots & \mathbb{I}_{m,n} a_m \mathbf{x}_n \end{pmatrix} \in \mathbb{R}^{md \times n},$$

and $\mathbf{H} = \mathbf{Z}^\top \mathbf{Z}$. Note that

$$\mathbf{H}_{ij} = \frac{\mathbf{x}_i^\top \mathbf{x}_j}{m} \sum_{r=1}^{m} \mathbb{I}_{r,i} \mathbb{I}_{r,j}, \quad \forall i, j \in [n].$$

With this notation we have a more compact form of the gradient (5):

$$\text{vec}\left(\nabla \Phi(\mathbf{W})\right) = \mathbf{Z}(\mathbf{u} - \mathbf{y}).$$

Then the GD update rule is:

$$\text{vec}\left(\mathbf{W}(k+1)\right) = \text{vec}\left(\mathbf{W}(k)\right) - \eta \mathbf{Z}(k)(\mathbf{u}(k) - y), \quad (6)$$

for $k = 0, 1, \ldots$. Throughout the paper, we use k as the iteration number, and also use k to index all variables that depend on $\mathbf{W}(k)$. For example, we have $u_i(k) = f_{\mathbf{W}(k),\mathbf{a}}(\mathbf{x}_i)$, $\mathbb{I}_{r,i}(k) = \mathbb{I}\left\{\mathbf{w}_r(k)^\top \mathbf{x}_i \geq 0\right\}$, etc.

4. Analysis of Convergence Rate

Although Theorem 3.1 already predicts linear convergence of GD to 0 loss, it only provides an upper bound on the loss and does not distinguish different types of labels. In particular, it cannot answer Question 1. In this section we give a fine-grained analysis of the convergence rate.

Recall the loss function $\Phi(\mathbf{W}) = \frac{1}{2}\left\|\mathbf{y} - \mathbf{u}\right\|_2^2$. Thus, it is equivalent to study how fast the sequence $\left\{\mathbf{u}(k)\right\}_{k=0}^{\infty}$ converges to $\mathbf{y}$. Key to our analysis is the observation that when the size of initialization κ is small and the network width m is large, the sequence $\left\{\mathbf{u}(k)\right\}_{k=0}^{\infty}$ stays close to another sequence $\left\{\tilde{\mathbf{u}}(k)\right\}_{k=0}^{\infty}$ which has a *linear* update rule:

$$\begin{aligned} \tilde{\mathbf{u}}(0) &= \mathbf{0}, \\ \tilde{\mathbf{u}}(k+1) &= \tilde{\mathbf{u}}(k) - \eta \mathbf{H}^\infty \left(\tilde{\mathbf{u}}(k) - \mathbf{y}\right), \end{aligned} \quad (7)$$

where $\mathbf{H}^\infty$ is the Gram matrix defined in (3).

Write the eigen-decomposition $\mathbf{H}^\infty = \sum_{i=1}^{n} \lambda_i \mathbf{v}_i \mathbf{v}_i^\top$, where $\mathbf{v}_1, \ldots, \mathbf{v}_n \in \mathbb{R}^n$ are orthonormal eigenvectors of $\mathbf{H}^\infty$ and $\lambda_1, \ldots, \lambda_n$ are corresponding eigenvalues. Our main theorem in this section is the following:

Theorem 4.1. *Suppose* $\lambda_0 = \lambda_{\min}(\mathbf{H}^\infty) > 0$, $\kappa = O\left(\frac{\epsilon\delta}{\sqrt{n}}\right)$, $m = \Omega\left(\frac{n^7}{\lambda_0^4 \kappa^2 \delta^4 \epsilon^2}\right)$ *and* $\eta = O\left(\frac{\lambda_0}{n^2}\right)$. *Then with probability at least* $1 - \delta$ *over the random initialization, for all* $k = 0, 1, 2, \ldots$ *we have:*

$$\left\|\mathbf{y} - \mathbf{u}(k)\right\|_2 = \sqrt{\sum_{i=1}^{n} (1 - \eta\lambda_i)^{2k} \left(\mathbf{v}_i^\top \mathbf{y}\right)^2} \pm \epsilon. \quad (8)$$

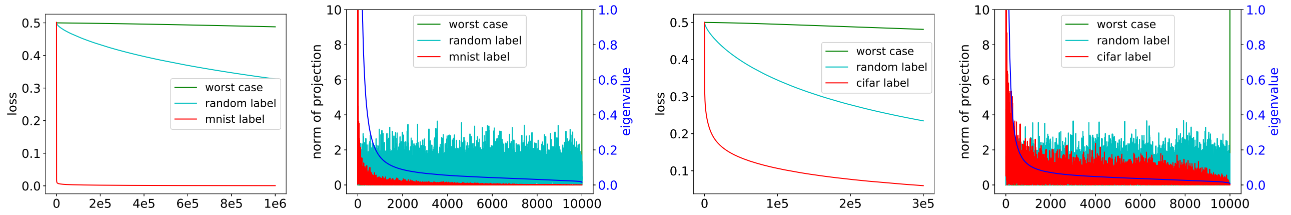
The proof of Theorem 4.1 is given in Appendix C.

In fact, the dominating term $\sqrt{\sum_{i=1}^{n} (1 - \eta\lambda_i)^{2k} \left(\mathbf{v}_i^\top \mathbf{y}\right)^2}$ is exactly equal to $\left\|\mathbf{y} - \tilde{\mathbf{u}}(k)\right\|_2$, which we prove in Section 4.1.

In light of (8), it suffices to understand how fast $\sum_{i=1}^{n} (1 - \eta\lambda_i)^{2k} \left(\mathbf{v}_i^\top \mathbf{y}\right)^2$ converges to 0 as k grows. Define $\xi_i(k) = (1 - \eta\lambda_i)^{2k} (\mathbf{v}_i^\top \mathbf{y})^2$, and notice that each sequence $\{\xi_i(k)\}_{k=0}^{\infty}$ is a geometric sequence which starts at $\xi_i(0) = (\mathbf{v}_i^\top \mathbf{y})^2$ and decreases at ratio $(1 - \eta\lambda_i)^2$. In other words, we can think of decomposing the label vector $\mathbf{y}$ into its projections onto all eigenvectors $\mathbf{v}_i$ of $\mathbf{H}^\infty$: $\|\mathbf{y}\|_2^2 = \sum_{i=1}^{n} (\mathbf{v}_i^\top \mathbf{y})^2 = \sum_{i=1}^{n} \xi_i(0)$, and the i-th portion shrinks exponentially at ratio $(1 - \eta\lambda_i)^2$. The larger λ_i is, the faster $\{\xi_i(k)\}_{k=0}^{\infty}$ decreases to 0, so in order to have faster convergence we would like the projections of $\mathbf{y}$ onto top eigenvectors to be larger. Therefore we obtain the following intuitive rule to compare the convergence rates on two sets of labels in a qualitative manner (for fixed $\|\mathbf{y}\|_2$):

- For a set of labels $\mathbf{y}$, if they align with the top eigenvectors, i.e., $(\mathbf{v}_i^\top \mathbf{y})^2$ is large for large λ_i, then gradient descent converges quickly.
- For a set of labels $\mathbf{y}$, if the projections on eigenvectors $\{(\mathbf{v}_i^\top \mathbf{y})^2\}_{i=1}^{n}$ are uniform, or labels align with eigenvectors with respect to small eigenvalues, then gradient descent converges with a slow rate.

Answer to Question 1. We now use this reasoning to answer Question 1. In Figure 1(b), we compute the eigenvalues of $\mathbf{H}^\infty$ (blue curve) for the MNIST dataset. The plot shows the eigenvalues of $\mathbf{H}^\infty$ admit a fast decay. We further compute the projections $\{|\mathbf{v}_i^\top \mathbf{y}|\}_{i=1}^{n}$ of true labels (red) and random labels (cyan). We observe that there is a significant difference between the projections of true labels and random labels: true labels align well with top eigenvectors whereas projections of random labels are close to being uniform. Furthermore, according to our theory, if a set of labels align with the eigenvector associated with the least eigenvalue, the convergence rate of gradient descent will be extremely slow. We construct such labels and in Figure 1(a) we indeed observe slow convergence. We repeat the same experiments on CIFAR and have similar observations (Figures 1(c) and



(a) Convergence Rate, MNIST. (b) Eigenval & Projections, MNIST. (c) Convergence Rate, CIFAR. (d) Eigenval & Projections, CIFAR.

Figure 1: In Figures 1(a) and 1(c), we compare convergence rates of gradient descent between using true labels, random labels and the worst case labels (normalized eigenvector of $\mathbf{H}^{\infty}$ corresponding to $\lambda_{\min}(\mathbf{H}^{\infty})$. In Figures 1(b) and 1(d), we plot the eigenvalues of $\mathbf{H}^{\infty}$ as well as projections of true, random, and worst case labels on different eigenvectors of $\mathbf{H}^{\infty}$. The experiments use gradient descent on data from two classes of MNIST or CIFAR. The plots clearly demonstrate that true labels have much better alignment with top eigenvectors, thus enjoying faster convergence.

1(d)). These empirical findings support our theory on the convergence rate of gradient descent. See Appendix A for implementation details.

4.1. Proof Sketch of Theorem 4.1

Now we prove $\|\mathbf{y}-\tilde{\mathbf{u}}(k)\|_2^2 = \sum_{i=1}^n (1-\eta\lambda_i)^{2k}\left(\mathbf{v}_i^\top \mathbf{y}\right)^2$. The entire proof of Theorem 4.1 is given in Appendix C, which relies on the fact that the dynamics of $\{\mathbf{u}(k)\}_{k=0}^{\infty}$ is essentially a perturbed version of (7).

From (7) we have $\tilde{\mathbf{u}}(k+1)-\mathbf{y} = (\mathbf{I}-\eta\mathbf{H}^{\infty})\left(\tilde{\mathbf{u}}(k)-\mathbf{y}\right)$, which implies $\tilde{\mathbf{u}}(k)-\mathbf{y} = (\mathbf{I}-\eta\mathbf{H}^{\infty})^k\left(\tilde{\mathbf{u}}(0)-\mathbf{y}\right) = -(\mathbf{I}-\eta\mathbf{H}^{\infty})^k\mathbf{y}$. Note that $(\mathbf{I}-\eta\mathbf{H}^{\infty})^k$ has eigendecomposition $(\mathbf{I}-\eta\mathbf{H}^{\infty})^k = \sum_{i=1}^n (1-\eta\lambda_i)^k \mathbf{v}_i\mathbf{v}_i^\top$ and that $\mathbf{y}$ can be decomposed as $\mathbf{y} = \sum_{i=1}^n (\mathbf{v}_i^\top\mathbf{y})\mathbf{v}_i$. Then we have $\tilde{\mathbf{u}}(k)-\mathbf{y} = -\sum_{i=1}^n (1-\eta\lambda_i)^k(\mathbf{v}_i^\top\mathbf{y})\mathbf{v}_i$, which implies $\|\tilde{\mathbf{u}}(k)-\mathbf{y}\|_2^2 = \sum_{i=1}^n (1-\eta\lambda_i)^{2k}(\mathbf{v}_i^\top\mathbf{y})^2$.

5. Analysis of Generalization

In this section, we study the generalization ability of the two-layer neural network $f_{\mathbf{W}(k),\mathbf{a}}$ trained by GD.

First, in order for optimization to succeed, i.e., zero training loss is achieved, we need a *non-degeneracy* assumption on the data distribution, defined below:

Definition 5.1. *A distribution $\mathcal{D}$ over $\mathbb{R}^d \times \mathbb{R}$ is (λ_0, δ, n)-non-degenerate, if for n i.i.d. samples $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ from $\mathcal{D}$, with probability at least $1-\delta$ we have $\lambda_{\min}(\mathbf{H}^{\infty}) \geq \lambda_0 > 0$.*

Remark 5.1. *Note that as long as no two $\mathbf{x}_i$ and $\mathbf{x}_j$ are parallel to each other, we have $\lambda_{\min}(\mathbf{H}^{\infty}) > 0$. (See (Du et al., 2018c)). For most real-world distributions, any two training inputs are not parallel.*

Our main theorem is the following:

Theorem 5.1. *Fix a failure probability $\delta \in (0,1)$. Suppose our data $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ are i.i.d. samples from a $(\lambda_0, \delta/3, n)$-non-degenerate distribution $\mathcal{D}$, and $\kappa = O\left(\frac{\lambda_0\delta}{n}\right), m \geq \kappa^{-2}\mathrm{poly}\left(n, \lambda_0^{-1}, \delta^{-1}\right)$. Consider any loss function $\ell : \mathbb{R}\times\mathbb{R} \to [0,1]$ that is 1-Lipschitz in the first argument such that $\ell(y,y) = 0$. Then with probability at least $1-\delta$ over the random initialization and the training samples, the two-layer neural network $f_{\mathbf{W}(k),\mathbf{a}}$ trained by GD for $k \geq \Omega\left(\frac{1}{\eta\lambda_0}\log\frac{n}{\delta}\right)$ iterations has population loss $L_{\mathcal{D}}(f_{\mathbf{W}(k),\mathbf{a}}) = \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell(f_{\mathbf{W}(k),\mathbf{a}}(\mathbf{x}), y)\right]$ bounded as:*

$$L_{\mathcal{D}}(f_{\mathbf{W}(k),\mathbf{a}}) \leq \sqrt{\frac{2\mathbf{y}^\top\left(\mathbf{H}^{\infty}\right)^{-1}\mathbf{y}}{n}} + O\left(\sqrt{\frac{\log\frac{n}{\lambda_0\delta}}{n}}\right). \tag{9}$$

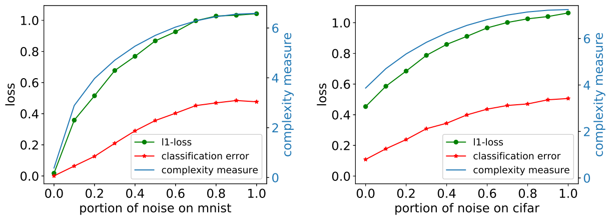
The proof of Theorem 5.1 is given in Appendix D and we sketch the proof in Section 5.1.

Note that in Theorem 5.1 there are three sources of possible failures: (i) failure of satisfying $\lambda_{\min}(\mathbf{H}^{\infty}) \geq \lambda_0$, (ii) failure of random initialization, and (iii) failure in the data sampling procedure (c.f. Theorem B.1). We ensure that all these failure probabilities are at most $\delta/3$ so that the final failure probability is at most δ.

As a corollary of Theorem 5.1, for binary classification problems (i.e., labels are ±1), we can show that (9) also bounds the *population classification error* of the learned classifier. See Appendix D for the proof.

Corollary 5.2. *Under the same assumptions as in Theorem 5.1 and additionally assuming that $y \in \{\pm 1\}$ for $(\mathbf{x}, y) \sim \mathcal{D}$, with probability at least $1-\delta$, the population classification error $L_{\mathcal{D}}^{01}(f_{\mathbf{W}(k),\mathbf{a}}) = \Pr_{(\mathbf{x},y)\sim\mathcal{D}}\left[\mathrm{sign}\left(f_{\mathbf{W}(k),\mathbf{a}}(\mathbf{x})\right) \neq y\right]$ is bounded as:*

$$L_{\mathcal{D}}^{01}(f_{\mathbf{W}(k),\mathbf{a}}) \leq \sqrt{\frac{2\mathbf{y}^\top\left(\mathbf{H}^{\infty}\right)^{-1}\mathbf{y}}{n}} + O\left(\sqrt{\frac{\log\frac{n}{\lambda_0\delta}}{n}}\right).$$



(a) MNIST Data. (b) CIFAR Data.

Figure 2: Generalization error (ℓ_1 loss and classification error) v.s. our complexity measure when different portions of random labels are used. We apply GD on data from two classes of MNIST or CIFAR until convergence. Our complexity measure almost matches the trend of generalization error as the portion of random labels increases. Note that ℓ_1 loss is always an upper bound on the classification error.

Now we discuss our generalization bound. The dominating term in (9) is:

$$\sqrt{\frac{2\mathbf{y}^\top \left(\mathbf{H}^\infty\right)^{-1}\mathbf{y}}{n}}. \tag{10}$$

This can be viewed as a *complexity measure of data* that one can use to predict the test accuracy of the learned neural network. Our result has the following advantages: (i) our complexity measure (10) can be directly computed given data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, without the need of training a neural network or assuming a ground-truth model; (ii) our bound is completely independent of the network width m.

Evaluating our completixy measure (10). To illustrate that the complexity measure in (10) effectively determines test error, in Figure 2 we compare this complexity measure versus the test error with true labels and random labels (and mixture of true and random labels). Random and true labels have significantly different complexity measures, and as the portion of random labels increases, our complexity measure also increases. See Appendix A for implementation details.

5.1. Proof Sketch of Theorem 5.1

The main ingredients in the proof of Theorem 5.1 are Lemmas 5.3 and 5.4. We defer the proofs of these lemmas as well as the full proof of Theorem 5.1 to Appendix D.

Our proof is based on a careful characterization of the trajectory of $\{\mathbf{W}(k)\}_{k=0}^\infty$ during GD. In particular, we bound its *distance to initialization* as follows:

Lemma 5.3. *Suppose* $m \ge \kappa^{-2}\mathrm{poly}\left(n, \lambda_0^{-1}, \delta^{-1}\right)$ *and* $\eta = O\left(\frac{\lambda_0}{n^2}\right)$. *Then with probability at least* $1-\delta$ *over the random initialization, we have for all* $k \ge 0$:

- $\left\|\mathbf{w}_r(k) - \mathbf{w}_r(0)\right\|_2 = O\left(\frac{n}{\sqrt{m}\lambda_0\sqrt{\delta}}\right)$ $(\forall r \in [m])$, *and*
- $\left\|\mathbf{W}(k) - \mathbf{W}(0)\right\|_F \le \sqrt{\mathbf{y}^\top\left(\mathbf{H}^\infty\right)^{-1}\mathbf{y}} + O\left(\frac{n\kappa}{\lambda_0\delta}\right) + \frac{\mathrm{poly}\left(n, \lambda_0^{-1}, \delta^{-1}\right)}{m^{1/4}\kappa^{1/2}}$.

The bound on the movement of each $\mathbf{w}_r$ was proved in (Du et al., 2018c). Our main contribution is the bound on $\left\|\mathbf{W}(k) - \mathbf{W}(0)\right\|_F$ which corresponds to the *total movement of all neurons*. The main idea is to couple the trajectory of $\{\mathbf{W}(k)\}_{k=0}^\infty$ with another simpler trajectory $\left\{\widetilde{\mathbf{W}}(k)\right\}_{k=0}^\infty$ defined as:

$$\widetilde{\mathbf{W}}(0) = \mathbf{0},$$

$$\mathrm{vec}\left(\widetilde{\mathbf{W}}(k+1)\right) = \mathrm{vec}\left(\widetilde{\mathbf{W}}(k)\right) - \eta\mathbf{Z}(0)\left(\mathbf{Z}(0)^\top\mathrm{vec}\left(\widetilde{\mathbf{W}}(k)\right) - \mathbf{y}\right). \tag{11}$$

We prove $\left\|\widetilde{\mathbf{W}}(\infty) - \widetilde{\mathbf{W}}(0)\right\|_F = \sqrt{\mathbf{y}^\top\mathbf{H}(0)^{-1}\mathbf{y}}$ in Section 5.2.[4] The actually proof of Lemma 5.3 is essentially a perturbed version of this.

Lemma 5.3 implies that the learned function $f_{\mathbf{W}(k),\mathbf{a}}$ from GD is in a *restricted* class of neural nets whose weights are close to initialization $\mathbf{W}(0)$. The following lemma bounds the Rademacher complexity of this function class:

Lemma 5.4. *Given* $R > 0$, *with probability at least* $1-\delta$ *over the random initialization* $(\mathbf{W}(0), \mathbf{a})$, *simultaneously for every* $B > 0$, *the following function class*

$$\mathcal{F}_{R,B}^{\mathbf{W}(0),\mathbf{a}} = \{f_{\mathbf{W},\mathbf{a}} : \left\|\mathbf{w}_r - \mathbf{w}_r(0)\right\|_2 \le R \; (\forall r \in [m]), \left\|\mathbf{W} - \mathbf{W}(0)\right\|_F \le B\}$$

has empirical Rademacher complexity bounded as:

$$\mathcal{R}_S\left(\mathcal{F}_{R,B}^{\mathbf{W}(0),\mathbf{a}}\right) = \frac{1}{n}\mathbb{E}_{\boldsymbol{\varepsilon}\in\{\pm1\}^n}\left[\sup_{f\in\mathcal{F}_{R,B}^{\mathbf{W}(0),\mathbf{a}}}\sum_{i=1}^n \varepsilon_i f(\mathbf{x}_i)\right]$$
$$\le \frac{B}{\sqrt{2n}}\left(1 + \left(\frac{2\log\frac{2}{\delta}}{m}\right)^{1/4}\right) + \frac{2R^2\sqrt{m}}{\kappa} + R\sqrt{2\log\frac{2}{\delta}}.$$

Finally, combining Lemmas 5.3 and 5.4, we are able to conclude that the neural network found by GD belongs to a function class with Rademacher complexity at most $\sqrt{\mathbf{y}^\top(\mathbf{H}^\infty)^{-1}\mathbf{y}/(2n)}$ (plus negligible errors). This gives us the generalization bound in Theorem 5.1 using the theory of Rademacher complexity (Appendix B).

5.2. Analysis of the Auxiliary Sequence $\left\{\widetilde{\mathbf{W}}(k)\right\}_{k=0}^\infty$

Now we give a proof of $\left\|\widetilde{\mathbf{W}}(\infty) - \widetilde{\mathbf{W}}(0)\right\|_F = \sqrt{\mathbf{y}^\top\mathbf{H}(0)^{-1}\mathbf{y}}$ as an illustration for the proof of Lemma 5.3.

[4] Note that we have $\mathbf{H}(0) \approx \mathbf{H}^\infty$ from standard concentration. See Lemma C.3.

Define $\mathbf{v}(k) = \mathbf{Z}(0)^\top \text{vec}\left(\widetilde{\mathbf{W}}(k)\right) \in \mathbb{R}^n$. Then from (11) we have $\mathbf{v}(0) = \mathbf{0}$ and $\mathbf{v}(k+1) = \mathbf{v}(k) - \eta\mathbf{H}(0)(\mathbf{v}(k) - \mathbf{y})$, yielding $\mathbf{v}(k) - \mathbf{y} = -(\mathbf{I} - \eta\mathbf{H}(0))^k\mathbf{y}$. Plugging this back to (11) we get $\text{vec}\left(\widetilde{\mathbf{W}}(k+1)\right) - \text{vec}\left(\widetilde{\mathbf{W}}(k)\right) = \eta\mathbf{Z}(0)(\mathbf{I} - \eta\mathbf{H}(0))^k\mathbf{y}$. Then taking a sum over $k = 0, 1, \ldots$ we have

$$\begin{aligned}\text{vec}\left(\widetilde{\mathbf{W}}(\infty)\right) - \text{vec}\left(\widetilde{\mathbf{W}}(0)\right) &= \sum_{k=0}^{\infty} \eta\mathbf{Z}(0)(\mathbf{I} - \eta\mathbf{H}(0))^k\mathbf{y} \\ &= \mathbf{Z}(0)\mathbf{H}(0)^{-1}\mathbf{y}.\end{aligned}$$

The desired result thus follows:

$$\begin{aligned}\left\|\widetilde{\mathbf{W}}(\infty) - \widetilde{\mathbf{W}}(0)\right\|_F^2 &= \mathbf{y}^\top\mathbf{H}(0)^{-1}\mathbf{Z}(0)^\top\mathbf{Z}(0)\mathbf{H}(0)^{-1}\mathbf{y} \\ &= \mathbf{y}^\top\mathbf{H}(0)^{-1}\mathbf{y}.\end{aligned}$$

6. Provable Learning using Two-Layer ReLU Neural Networks

Theorem 5.1 determines that $\sqrt{\frac{2\mathbf{y}^\top(\mathbf{H}^\infty)^{-1}\mathbf{y}}{n}}$ controls the generalization error. In this section, we study what functions can be provably learned in this setting. We assume the data satisfy $y_i = g(\mathbf{x}_i)$ for some underlying function $g : \mathbb{R}^d \to \mathbb{R}$. A simple observation is that if we can prove

$$\mathbf{y}^\top(\mathbf{H}^\infty)^{-1}\mathbf{y} \le M_g$$

for some quantity M_g that is *independent* of the number of samples n, then Theorem 5.1 implies we can provably learn the function g on the underlying data distribution using $O\left(\frac{M_g + \log(1/\delta)}{\epsilon^2}\right)$ samples. The following theorem shows that this is indeed the case for a broad class of functions.

Theorem 6.1. *Suppose we have*

$$y_i = g(\mathbf{x}_i) = \alpha\left(\boldsymbol{\beta}^\top\mathbf{x}_i\right)^p, \quad \forall i \in [n],$$

where $p = 1$ or $p = 2l$ ($l \in \mathbb{N}_+$), $\boldsymbol{\beta} \in \mathbb{R}^d$ and $\alpha \in \mathbb{R}$. Then we have

$$\sqrt{\mathbf{y}^\top(\mathbf{H}^\infty)^{-1}\mathbf{y}} \le 3p\,|\alpha| \cdot \|\boldsymbol{\beta}\|_2^p\,.$$

The proof of Theorem 6.1 is given in Appendix E.

Notice that for two label vectors $\mathbf{y}^{(1)}$ and $\mathbf{y}^{(2)}$, we have

$$\begin{aligned}&\sqrt{(\mathbf{y}^{(1)} + \mathbf{y}^{(2)})^\top(\mathbf{H}^\infty)^{-1}\left(\mathbf{y}^{(1)} + \mathbf{y}^{(2)}\right)} \\ \le &\sqrt{(\mathbf{y}^{(1)})^\top(\mathbf{H}^\infty)^{-1}\mathbf{y}^{(1)}} + \sqrt{(\mathbf{y}^{(2)})^\top(\mathbf{H}^\infty)^{-1}\mathbf{y}^{(2)}}.\end{aligned}$$

This implies that *the sum of learnable functions is also learnable*. Therefore, the following is a direct corollary of Theorem 6.1:

Corollary 6.2. *Suppose we have*

$$y_i = g(\mathbf{x}_i) = \sum_j \alpha_j\left(\boldsymbol{\beta}_j^\top\mathbf{x}_i\right)^{p_j}, \quad \forall i \in [n], \tag{12}$$

where for each j, $p_j \in \{1, 2, 4, 6, 8, \ldots\}$, $\boldsymbol{\beta}_j \in \mathbb{R}^d$ and $\alpha_j \in \mathbb{R}$. Then we have

$$\sqrt{\mathbf{y}^\top(\mathbf{H}^\infty)^{-1}\mathbf{y}} \le 3\sum_j p_j\,|\alpha_j| \cdot \|\boldsymbol{\beta}_j\|_2^{p_j}\,. \tag{13}$$

Corollary 6.2 shows that overparameterized two-layer ReLU network can learn any function of the form (12) for which (13) is bounded. One can view (12) as two-layer neural networks with polynomial activation $\phi(z) = z^p$, where $\{\boldsymbol{\beta}_j\}$ are weights in the first layer and $\{\alpha_j\}$ are the second layer. Below we give some specific examples.

Example 6.1 (Linear functions)**.** *For $g(\mathbf{x}) = \boldsymbol{\beta}^\top\mathbf{x}$, we have $M_g = O(\|\boldsymbol{\beta}\|_2^2)$.*

Example 6.2 (Quadratic functions)**.** *For $g(\mathbf{x}) = \mathbf{x}^\top\mathbf{A}\mathbf{x}$ where $\mathbf{A} \in \mathbb{R}^{d\times d}$ is symmetric, we can write down the eigen-decomposition $\mathbf{A} = \sum_{j=1}^d \alpha_j\boldsymbol{\beta}_j\boldsymbol{\beta}_j^\top$. Then we have $g(\mathbf{x}) = \sum_{j=1}^d \alpha_j(\boldsymbol{\beta}_j^\top\mathbf{x})^2$, so $M_g = O\left(\sum_{i=1}^d |\alpha_j|\right) = O(\|\mathbf{A}\|_*)$.*[5] *This is also the class of two-layer neural networks with quadratic activation.*

Example 6.3 (Cosine activation)**.** *Suppose $g(\mathbf{x}) = \cos(\boldsymbol{\beta}^\top\mathbf{x}) - 1$ for some $\boldsymbol{\beta} \in \mathbb{R}^d$. Using Taylor series we know $g(\mathbf{x}) = \sum_{j=1}^\infty \frac{(-1)^j(\boldsymbol{\beta}^\top\mathbf{x})^{2j}}{(2j)!}$. Thus we have $M_g = O\left(\sum_{j=1}^\infty \frac{j}{(2j)!}\|\boldsymbol{\beta}\|_2^{2j}\right) = O\left(\|\boldsymbol{\beta}\|_2 \cdot \sinh(\|\boldsymbol{\beta}\|_2)\right)$.*

Finally, we note that our "smoothness" requirement (13) is weaker than that in (Allen-Zhu et al., 2018a), as illustrated in the following example.

Example 6.4 (A not-so-smooth function)**.** *Suppose $g(\mathbf{x}) = \phi(\boldsymbol{\beta}^\top\mathbf{x})$, where $\phi(z) = z \cdot \arctan(\frac{z}{2})$ and $\|\boldsymbol{\beta}\|_2 \le 1$. We have $g(\mathbf{x}) = \sum_{j=1}^\infty \frac{(-1)^{j-1}2^{1-2j}}{2j-1}\left(\boldsymbol{\beta}^\top\mathbf{x}\right)^{2j}$ since $\left|\boldsymbol{\beta}^\top\mathbf{x}\right| \le 1$. Thus $M_g = O\left(\sum_{j=1}^\infty \frac{j\cdot 2^{1-2j}}{2j-1}\|\boldsymbol{\beta}\|_2^{2j}\right) \le O\left(\sum_{j=1}^\infty 2^{1-2j}\|\boldsymbol{\beta}\|^{2j}\right) = O\left(\|\boldsymbol{\beta}\|_2^2\right)$, so our result implies that this function is learnable by 2-layer ReLU nets.*

However, Allen-Zhu et al. (2018a)'s generalization theorem would require $\sum_{j=1}^\infty \frac{\left(C\sqrt{\log(1/\epsilon)}\right)^{2j}2^{1-2j}}{2j-1}$ to be bounded, where C is a large constant and ϵ is the target generalization error. This is clearly not satisfied.

7. Conclusion

This paper shows how to give a fine-grained analysis of the optimization trajectory and the generalization ability of overparameterized two-layer neural networks trained by gradient descent. We believe that our approach can also be useful in analyzing overparameterized deep neural networks and other machine learning models.

[5] $\|\mathbf{A}\|_*$ is the trace-norm of $\mathbf{A}$.

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Appendix

A. Experiment Setup

The architecture of our neural networks is as described in Section 3.1. During the training process, we fix the second layer and only optimize the first layer, following the setting in Section 3.1. We fix the number of neurons to be $m = 10,000$ in all experiments. We train the neural network using (full-batch) gradient descent (GD), with a fixed learning rate $\eta = 10^{-3}$. Our theory requires a small scaling factor κ during the initialization (cf. (1)). We fix $\kappa = 10^{-2}$ in all experiments. We train the neural networks until the training ℓ_2 loss converges.

We use two image datasets, the CIFAR dataset (Krizhevsky & Hinton, 2009) and the MNIST dataset (LeCun et al., 1998), in our experiments. We only use the first two classes of images in the the CIFAR dataset and the MNIST dataset, with $10,000$ training images and $2,000$ validation images in total for each dataset. In both datasets, for each image $\mathbf{x}_i$, we set the corresponding label y_i to be $+1$ if the image belongs to the first class, and -1 otherwise. For each image $\mathbf{x}_i$ in the dataset, we normalize the image so that $\|\mathbf{x}_i\|_2 = 1$, following the setup in Section 3.1.

In the experiments reported in Figure 2, we choose a specific portion of (both training and test) data uniformly at random, and change their labels y_i to $\mathrm{unif}\left(\{-1, 1\}\right)$.

Our neural networks are trained using the PyTorch package (Paszke et al., 2017), using (possibly multiple) NVIDIA Tesla V100 GPUs.

B. Background on Generalization and Rademacher Complexity

Consider a loss function $\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$. For a function $f : \mathbb{R}^d \to \mathbb{R}$, the *population loss* over data distribution $\mathcal{D}$ as well as the *empirical loss* over n samples $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ from $\mathcal{D}$ are defined as:

$$L_\mathcal{D}(f) = \mathop{\mathbb{E}}_{(\mathbf{x},y)\sim\mathcal{D}} \left[\ell(f(\mathbf{x}), y)\right],$$

$$L_S(f) = \frac{1}{n}\sum_{i=1}^n \ell(f(\mathbf{x}_i), y_i).$$

Generalization error refers to the gap $L_\mathcal{D}(f) - L_S(f)$ for the learned function f given sample S.

Recall the standard definition of Rademacher complexity:

Definition B.1. *Given n samples S, the empirical Rademacher complexity of a function class $\mathcal{F}$ (mapping from $\mathbb{R}^d$ to $\mathbb{R}$) is defined as:*

$$\mathcal{R}_S(\mathcal{F}) = \frac{1}{n}\mathbb{E}_{\boldsymbol{\varepsilon}}\left[\sup_{f\in\mathcal{F}}\sum_{i=1}^n \varepsilon_i f(\mathbf{x}_i)\right],$$

where $\boldsymbol{\varepsilon} = (\varepsilon_1, \ldots, \varepsilon_n)^\top$ contains i.i.d. random variables drawn from the Rademacher distribution $\mathrm{unif}(\{1, -1\})$.

Rademacher complexity directly gives an upper bound on generalization error (see e.g. (Mohri et al., 2012)):

Theorem B.1. *Suppose the loss function $\ell(\cdot,\cdot)$ is bounded in $[0, c]$ and is ρ-Lipschitz in the first argument. Then with probability at least $1-\delta$ over sample S of size n:*

$$\sup_{f\in\mathcal{F}}\left\{L_\mathcal{D}(f) - L_S(f)\right\} \le 2\rho\mathcal{R}_S(\mathcal{F}) + 3c\sqrt{\frac{\log(2/\delta)}{2n}}.$$

Therefore, as long as we can bound the Rademacher complexity of a certain function class that contains our learned predictor, we can obtain a generalization bound.

C. Proofs for Section 4

In this section we prove Theorem 4.1.

We first show some technical lemmas. Most of them are already proved in (Du et al., 2018c) and we give proofs for them for completeness.

First, we have the following lemma which gives an upper bound on how much each weight vector can move during optimization.

Lemma C.1. *Under the same setting as Theorem 3.1, i.e.,* $\lambda_0 = \lambda_{\min}(\mathbf{H}^\infty) > 0$*,* $m = \Omega\left(\frac{n^6}{\lambda_0^4 \kappa^2 \delta^3}\right)$ *and* $\eta = O\left(\frac{\lambda_0}{n^2}\right)$*, with probability at least* $1-\delta$ *over the random initialization we have*

$$\|\mathbf{w}_r(k) - \mathbf{w}_r(0)\|_2 \le \frac{4\sqrt{n}\,\|\mathbf{y}-\mathbf{u}(0)\|_2}{\sqrt{m}\lambda_0}, \quad \forall r \in [m], \forall k \ge 0.$$

Proof. From Theorem 3.1 we know $\|\mathbf{y}-\mathbf{u}(k+1)\|_2 \le \sqrt{1-\frac{\eta\lambda_0}{2}}\,\|\mathbf{y}-\mathbf{u}(k)\|_2 \le \left(1-\frac{\eta\lambda_0}{4}\right)\|\mathbf{y}-\mathbf{u}(k)\|_2$ for all $k \ge 0$, which implies

$$\|\mathbf{y}-\mathbf{u}(k)\|_2 \le \left(1-\frac{\eta\lambda_0}{4}\right)^k \|\mathbf{y}-\mathbf{u}(0)\|_2\,, \quad \forall k \ge 0. \tag{14}$$

Recall the GD update rule:

$$\mathbf{w}_r(k+1) - \mathbf{w}_r(k) = -\eta \frac{\partial \Phi(\mathbf{W})}{\partial \mathbf{w}_r}\bigg|_{\mathbf{W}=\mathbf{W}(k)} = -\frac{\eta}{\sqrt{m}} a_r \sum_{i=1}^n (u_i(k)-y_i)\mathbb{I}_{r,i}(k)\mathbf{x}_i,$$

which implies

$$\|\mathbf{w}_r(k+1) - \mathbf{w}_r(k)\|_2 \le \frac{\eta}{\sqrt{m}} \sum_{i=1}^n |u_i(k)-y_i| \le \frac{\eta\sqrt{n}}{\sqrt{m}} \|\mathbf{y}-\mathbf{u}(k)\|_2\,.$$

Therefore, we have

$$\begin{aligned}
\|\mathbf{w}_r(k) - \mathbf{w}_r(0)\|_2 &\le \sum_{t=0}^{k-1} \|\mathbf{w}_r(t+1) - \mathbf{w}_r(t)\|_2 \\
&\le \sum_{t=0}^{k-1} \frac{\eta\sqrt{n}}{\sqrt{m}} \|\mathbf{y}-\mathbf{u}(k)\|_2 \\
&\le \frac{\eta\sqrt{n}}{\sqrt{m}} \sum_{t=0}^{\infty} \left(1-\frac{\eta\lambda_0}{4}\right)^k \|\mathbf{y}-\mathbf{u}(0)\|_2 \\
&= \frac{4\sqrt{n}\,\|\mathbf{y}-\mathbf{u}(0)\|_2}{\sqrt{m}\lambda_0},
\end{aligned}$$

completing the proof. □

As a consequence of Lemma C.1, we can upper bound the norms of $\mathbf{H}(k) - \mathbf{H}(0)$ and $\mathbf{Z}(k) - \mathbf{Z}(0)$ for all k. These bounds show that the matrices $\mathbf{H}$ and $\mathbf{Z}$ do not change much during optimization if m is sufficiently large.

Lemma C.2. *Under the same setting as Theorem 3.1, with probability at least* $1-4\delta$ *over the random initialization, for all* $k \ge 0$ *we have:*

$$\begin{aligned}
\|\mathbf{H}(k) - \mathbf{H}(0)\|_F &= O\left(\frac{n^3}{\sqrt{m}\lambda_0\kappa\delta^{3/2}}\right), \\
\|\mathbf{Z}(k) - \mathbf{Z}(0)\|_F &= O\left(\frac{n}{\sqrt{m^{1/2}\lambda_0\kappa\delta^{3/2}}}\right).
\end{aligned}$$

Proof. Let $R = \frac{Cn}{\sqrt{m}\lambda_0\sqrt{\delta}}$ for some universal constant $C > 0$. From Lemma C.1 we know that with probability at least $1-\delta$ we have $\|\mathbf{w}_r(k) - \mathbf{w}_r(0)\| \le R$ for all $r \in [m]$ and all $k \ge 0$.

We define events

$$A_{r,i} = \left\{ \left| \mathbf{w}_r(0)^\top \mathbf{x}_i \right| \le R \right\}, \quad i \in [n], r \in [m]. \tag{15}$$

Then it is easy to see that

$$\mathbb{I}\left\{ \mathbb{I}_{r,i}(k) \neq \mathbb{I}_{r,i}(0) \right\} \le \mathbb{I}\{A_{r,i}\} + \mathbb{I}\{\|\mathbf{w}_r(k) - \mathbf{w}_r(0)\| > R\}, \quad \forall i \in [n], \forall r \in [m], \forall k \ge 0.$$

Then for any $i, j \in [n]$ we have

$$\begin{aligned} |\mathbf{H}_{ij}(k) - \mathbf{H}_{ij}(0)| &= \left| \frac{\mathbf{x}_i^\top \mathbf{x}_j}{m} \sum_{r=1}^m \left(\mathbb{I}_{r,i}(k)\mathbb{I}_{r,j}(k) - \mathbb{I}_{r,i}(0)\mathbb{I}_{r,j}(0) \right) \right| \\ &\le \frac{1}{m} \sum_{r=1}^m \left(\mathbb{I}\left\{ \mathbb{I}_{r,i}(k) \neq \mathbb{I}_{r,i}(0) \right\} + \mathbb{I}\left\{ \mathbb{I}_{r,j}(k) \neq \mathbb{I}_{r,j}(0) \right\} \right) \\ &\le \frac{1}{m} \sum_{r=1}^m \left(\mathbb{I}\{A_{r,i}\} + \mathbb{I}\{A_{r,j}\} + 2\mathbb{I}\{\|\mathbf{w}_r(k) - \mathbf{w}_r(0)\| > R\} \right). \end{aligned} \tag{16}$$

Next, notice that $\mathbf{w}_r(0)^\top \mathbf{x}_i$ has the same distribution as $\mathcal{N}(0, \kappa^2)$. So we have

$$\mathbb{E}[\mathbb{I}\{A_{r,i}\}] = \Pr_{z \sim \mathcal{N}(0,\kappa^2)} [|z| \le R] = \int_{-R}^{R} \frac{1}{\sqrt{2\pi}\kappa} e^{-x^2/2\kappa^2} dx \le \frac{2R}{\sqrt{2\pi}\kappa}. \tag{17}$$

Now taking the expectation of (16), we have

$$\begin{aligned} \mathbb{E}\left[|\mathbf{H}_{ij}(k) - \mathbf{H}_{ij}(0)| \right] &\le \frac{1}{m} \sum_{r=1}^m \left(\mathbb{E}[\mathbb{I}\{A_{r,i}\}] + \mathbb{E}[\mathbb{I}\{A_{r,j}\}] + 2\mathbb{I}\{\|\mathbf{w}_r(k) - \mathbf{w}_r(0)\| > R\} \right) \\ &\le \frac{4R}{\sqrt{2\pi}\kappa} + \frac{2}{m} \sum_{r=1}^m \mathbb{E}\left[\mathbb{I}\{\|\mathbf{w}_r(k) - \mathbf{w}_r(0)\| > R\} \right] \\ &\le \frac{4R}{\sqrt{2\pi}\kappa} + \frac{2}{m}\delta, \qquad \forall i, j \in [n], \end{aligned}$$

which implies

$$\mathbb{E}\left[\|\mathbf{H}(k) - \mathbf{H}(0)\|_F \right] \le \mathbb{E}\left[\sum_{i,j=1}^n |\mathbf{H}_{ij}(k) - \mathbf{H}_{ij}(0)| \right] \le \frac{4n^2 R}{\sqrt{2\pi}\kappa} + \frac{2n^2\delta}{m}.$$

Then from Markov's inequality we know that with probability at least $1 - \delta$ we have $\|\mathbf{H}(k) - \mathbf{H}(0)\|_F \le \frac{4n^2 R}{\sqrt{2\pi}\kappa\delta} + \frac{2n^2}{m} = O\left(\frac{n^3}{\sqrt{m}\lambda_0 \kappa \delta^{3/2}} \right)$.

To bound $\|\mathbf{Z}(k) - \mathbf{Z}(0)\|_F$, we have

$$\begin{aligned} \mathbb{E}\left[\|\mathbf{Z}(k) - \mathbf{Z}(0)\|_F^2 \right] &= \mathbb{E}\left[\frac{1}{m} \sum_{i=1}^n \sum_{r=1}^m \left(\mathbb{I}_{r,i}(k) - \mathbb{I}_{r,i}(0) \right)^2 \right] \\ &= \frac{1}{m} \sum_{i=1}^n \sum_{r=1}^m \mathbb{E}\left[\mathbb{I}\{\mathbb{I}_{r,i}(k) \neq \mathbb{I}_{r,i}(0)\} \right] \\ &\le \frac{1}{m} \sum_{i=1}^n \sum_{r=1}^m \mathbb{E}\left[\mathbb{I}\{A_{r,i}\} + \mathbb{I}\{\|\mathbf{w}_r(k) - \mathbf{w}_r(0)\| > R\} \right] \\ &\le \frac{1}{m} \cdot mn \cdot \frac{2R}{\sqrt{2\pi}\kappa} + \frac{n}{m}\delta \\ &= \frac{2nR}{\sqrt{2\pi}\kappa} + \frac{n\delta}{m}. \end{aligned}$$

Using Markov's inequality, with probability at least $1 - \delta$ we have $\|\mathbf{Z}(k) - \mathbf{Z}(0)\|_F^2 \le \frac{2nR}{\sqrt{2\pi}\kappa\delta} + \frac{n}{m} = O\left(\frac{n^2}{\sqrt{m}\lambda_0 \kappa \delta^{3/2}} \right)$, proving the second part of the lemma. □

The next lemma shows that $\mathbf{H}(0)$ is close to $\mathbf{H}^\infty$.

Lemma C.3. *With probability at least* $1-\delta$*, we have* $\left\|\mathbf{H}(0)-\mathbf{H}^\infty\right\|_F = O\left(\frac{n\sqrt{\log\frac{n}{\delta}}}{\sqrt{m}}\right)$.

Proof. For all $i,j\in[n]$, $\mathbf{H}_{ij}(0)=\frac{\mathbf{x}_i^\top\mathbf{x}_j}{m}\sum_{r=1}^m \mathbb{I}_{r,i}(0)\mathbb{I}_{r,j}(0)$ is the average of m i.i.d. random variables bounded in $[0,1]$ with expectation $\mathbf{H}_{ij}^\infty$. Thus by Hoeffding's inequality, with probability at least $1-\delta'$ we have

$$\left|\mathbf{H}_{ij}(0)-\mathbf{H}_{ij}^\infty\right| \le \sqrt{\frac{\log(2/\delta')}{2m}}.$$

Letting $\delta'=\delta/n^2$ and applying a union bound over all $i,j\in[n]$, we know that with probability at least $1-\delta$:

$$\left\|\mathbf{H}(0)-\mathbf{H}^\infty\right\|_F^2 \le n^2\cdot\frac{\log(2n^2/\delta)}{2m}.$$

This completes the proof. □

Now we are ready to prove Theorem 4.1.

Proof of Theorem 4.1. We assume that all the high-probability ("with probability $1-\delta$") events happen. By a union bound at the end, the success probability is at least $1-\Omega(\delta)$, and then we can rescale δ by a constant such that the success probability is at least $1-\delta$.

The main idea is to show that the dynamics of $\{\mathbf{u}(k)\}_{k=0}^\infty$ is close to that of $\{\tilde{\mathbf{u}}(k)\}_{k=0}^\infty$. We have

$$u_i(k+1)-u_i(k)=\frac{1}{\sqrt{m}}\sum_{r=1}^m a_r\left[\sigma\left(\mathbf{w}_r(k+1)^\top\mathbf{x}_i\right)-\sigma\left(\mathbf{w}_r(k)^\top\mathbf{x}_i\right)\right]. \tag{18}$$

For each $i\in[n]$, we partition all m neurons into two parts:

$$S_i=\{r\in[m]:\mathbb{I}\{A_{r,i}\}=0\}$$

and

$$\bar{S}_i=\{r\in[m]:\mathbb{I}\{A_{r,i}\}=1\},$$

where $A_{r,i}$ is defined in (15). We know from the proof of Lemma C.2 that all neurons in S_i will not change activation pattern on data-point $\mathbf{x}_i$ during optimization, i.e.,

$$r\in S_i \Longrightarrow \mathbb{I}_{r,i}(k)=\mathbb{I}_{r,i}(0), \forall k\ge 0.$$

From (17) we know

$$\mathbb{E}\left[|\bar{S}_i|\right]=\mathbb{E}\left[\sum_{r=1}^m \mathbb{I}\{A_{r,i}\}\right]\le\frac{8\sqrt{mn}\left\|\mathbf{y}-\mathbf{u}(0)\right\|_2}{\sqrt{2\pi}\kappa\lambda_0}=O\left(\frac{\sqrt{m}n}{\kappa\lambda_0\sqrt{\delta}}\right),$$

where we have used $\left\|\mathbf{y}-\mathbf{u}(0)\right\|_2=O(\sqrt{n/\delta})$ (Theorem 3.1). Then we know $\mathbb{E}\left[\sum_{i=1}^n|\bar{S}_i|\right]=O\left(\frac{\sqrt{m}n^2}{\kappa\lambda_0\sqrt{\delta}}\right)$. Therefore with probability at least $1-\delta$ we have

$$\sum_{i=1}^n|\bar{S}_i|=O\left(\frac{\sqrt{m}n^2}{\kappa\lambda_0\delta^{3/2}}\right). \tag{19}$$

We write (18) as

$$\begin{aligned}&u_i(k+1)-u_i(k)\\=&\frac{1}{\sqrt{m}}\sum_{r\in S_i}a_r\left[\sigma\left(\mathbf{w}_r(k+1)^\top\mathbf{x}_i\right)-\sigma\left(\mathbf{w}_r(k)^\top\mathbf{x}_i\right)\right]+\frac{1}{\sqrt{m}}\sum_{r\in\bar{S}_i}a_r\left[\sigma\left(\mathbf{w}_r(k+1)^\top\mathbf{x}_i\right)-\sigma\left(\mathbf{w}_r(k)^\top\mathbf{x}_i\right)\right].\end{aligned} \tag{20}$$

We consider the two terms in (20) separately. We denote the second term as $\epsilon_i(k)$ and treat it as a perturbation term, which we bound as

$$\begin{aligned}
|\epsilon_i(k)| &= \left| \frac{1}{\sqrt{m}} \sum_{r \in \bar{S}_i} a_r \left[\sigma\left(\mathbf{w}_r(k+1)^\top \mathbf{x}_i\right) - \sigma\left(\mathbf{w}_r(k)^\top \mathbf{x}_i\right) \right] \right| \\
&\le \frac{1}{\sqrt{m}} \sum_{r \in \bar{S}_i} \left| \mathbf{w}_r(k+1)^\top \mathbf{x}_i - \mathbf{w}_r(k)^\top \mathbf{x}_i \right| \\
&\le \frac{1}{\sqrt{m}} \sum_{r \in \bar{S}_i} \left\| \mathbf{w}_r(k+1) - \mathbf{w}_r(k) \right\|_2 \\
&= \frac{1}{\sqrt{m}} \sum_{r \in \bar{S}_i} \left\| \frac{\eta}{\sqrt{m}} a_r \sum_{j=1}^n (u_j(k) - y_j) \mathbb{I}_{r,j}(k) \mathbf{x}_j \right\|_2 \\
&\le \frac{\eta}{m} \sum_{r \in \bar{S}_i} \sum_{j=1}^n |u_j(k) - y_j| \\
&\le \frac{\eta \sqrt{n} |\bar{S}_i|}{m} \left\| \mathbf{u}(k) - \mathbf{y} \right\|_2 .
\end{aligned} \tag{21}$$

For the first term in (20), we have

$$\begin{aligned}
&\frac{1}{\sqrt{m}} \sum_{r \in S_i} a_r \left[\sigma\left(\mathbf{w}_r(k+1)^\top \mathbf{x}_i\right) - \sigma\left(\mathbf{w}_r(k)^\top \mathbf{x}_i\right) \right] \\
=& \frac{1}{\sqrt{m}} \sum_{r \in S_i} a_r \mathbb{I}_{r,i}(k) \left(\mathbf{w}_r(k+1) - \mathbf{w}_r(k) \right)^\top \mathbf{x}_i \\
=& \frac{1}{\sqrt{m}} \sum_{r \in S_i} a_r \mathbb{I}_{r,i}(k) \left(-\frac{\eta}{\sqrt{m}} a_r \sum_{j=1}^n (u_j(k) - y_j) \mathbb{I}_{r,j}(k) \mathbf{x}_j \right)^\top \mathbf{x}_i \\
=& -\frac{\eta}{m} \sum_{j=1}^n (u_j(k) - y_j) \mathbf{x}_j^\top \mathbf{x}_i \sum_{r \in S_i} \mathbb{I}_{r,i}(k) \mathbb{I}_{r,j}(k) \\
=& -\eta \sum_{j=1}^n (u_j(k) - y_j) \mathbf{H}_{ij}(k) + \epsilon_i'(k),
\end{aligned} \tag{22}$$

where $\epsilon_i'(k) = \frac{\eta}{m} \sum_{j=1}^n (u_j(k) - y_j) \mathbf{x}_j^\top \mathbf{x}_i \sum_{r \in \bar{S}_i} \mathbb{I}_{r,i}(k) \mathbb{I}_{r,j}(k)$ is regarded as perturbation:

$$|\epsilon_i'(k)| \le \frac{\eta}{m} \left| \bar{S}_i \right| \sum_{j=1}^n |u_j(k) - y_j| \le \frac{\eta \sqrt{n} \left| \bar{S}_i \right|}{m} \left\| \mathbf{u}(k) - \mathbf{y} \right\|_2 . \tag{23}$$

Combining (20), (21), (22), (23), we have

$$u_i(k+1) - u_i(k) = -\eta \sum_{j=1}^n (u_j(k) - y_j) \mathbf{H}_{ij}(k) + \epsilon_i'(k) + \epsilon_i(k),$$

which gives

$$\mathbf{u}(k+1) - \mathbf{u}(k) = -\eta \mathbf{H}(k) (\mathbf{u}(k) - \mathbf{y}) + \boldsymbol{\epsilon}(k), \tag{24}$$

where $\boldsymbol{\epsilon}(k) \in \mathbb{R}^n$ can be bounded as

$$\begin{aligned}
\left\| \boldsymbol{\epsilon}(k) \right\|_2 \le \left\| \boldsymbol{\epsilon}(k) \right\|_1 = \sum_{i=1}^n |\epsilon_i(k) + \epsilon_i'(k)| \le \sum_{i=1}^n \frac{2\eta \sqrt{n} |\bar{S}_i|}{m} \left\| \mathbf{u}(k) - \mathbf{y} \right\|_2 = O\left(\frac{\sqrt{m} n^2}{\kappa \lambda_0 \delta^{3/2}} \right) \frac{2\eta \sqrt{n}}{m} \left\| \mathbf{u}(k) - \mathbf{y} \right\|_2 \\
= O\left(\frac{\eta n^{5/2}}{\sqrt{m} \kappa \lambda_0 \delta^{3/2}} \right) \left\| \mathbf{u}(k) - \mathbf{y} \right\|_2 .
\end{aligned}$$

Here we have used (19).

Next, since $\mathbf{H}(k)$ is close to $\mathbf{H}^\infty$ according to Lemmas C.2 and C.3, we rewrite (24) as

$$\mathbf{u}(k+1) - \mathbf{u}(k) = -\eta \mathbf{H}^\infty(\mathbf{u}(k) - \mathbf{y}) + \boldsymbol{\zeta}(k), \tag{25}$$

where $\boldsymbol{\zeta}(k) = \eta(\mathbf{H}^\infty - \mathbf{H}(k))(\mathbf{u}(k) - \mathbf{y}) + \boldsymbol{\epsilon}(k)$. From Lemmas C.2 and C.3 we have

$$\begin{aligned}\left\|\mathbf{H}^\infty - \mathbf{H}(k)\right\|_2 &\le \left\|\mathbf{H}^\infty - \mathbf{H}(k)\right\|_F \le \left\|\mathbf{H}(0) - \mathbf{H}(k)\right\|_F + \left\|\mathbf{H}(0) - \mathbf{H}^\infty\right\|_2 \\ &= O\left(\frac{n^3}{\sqrt{m}\lambda_0\kappa\delta^{3/2}}\right) + O\left(\frac{n\sqrt{\log\frac{n}{\delta}}}{\sqrt{m}}\right) = O\left(\frac{n^3}{\sqrt{m}\lambda_0\kappa\delta^{3/2}}\right).\end{aligned}$$

Therefore we can bound $\boldsymbol{\zeta}(k)$ as

$$\begin{aligned}\left\|\boldsymbol{\zeta}(k)\right\|_2 &\le \eta\left\|\mathbf{H}^\infty - \mathbf{H}(k)\right\|_2\left\|\mathbf{u}(k) - \mathbf{y}\right\|_2 + \left\|\boldsymbol{\epsilon}(k)\right\|_2 \\ &= O\left(\frac{\eta n^3}{\sqrt{m}\lambda_0\kappa\delta^{3/2}}\right)\left\|\mathbf{u}(k) - \mathbf{y}\right\|_2 + O\left(\frac{\eta n^{5/2}}{\sqrt{m}\kappa\lambda_0\delta^{3/2}}\right)\left\|\mathbf{u}(k) - \mathbf{y}\right\|_2 \\ &= O\left(\frac{\eta n^3}{\sqrt{m}\lambda_0\kappa\delta^{3/2}}\right)\left\|\mathbf{u}(k) - \mathbf{y}\right\|_2.\end{aligned} \tag{26}$$

Finally, applying (25) recursively, we get

$$\begin{aligned}\mathbf{u}(k) - \mathbf{y} &= (\mathbf{I} - \eta\mathbf{H}^\infty)^k(\mathbf{u}(0) - \mathbf{y}) + \sum_{t=0}^{k-1}(\mathbf{I} - \eta\mathbf{H}^\infty)^t\boldsymbol{\zeta}(k-1-t) \\ &= -(\mathbf{I} - \eta\mathbf{H}^\infty)^k\mathbf{y} + (\mathbf{I} - \eta\mathbf{H}^\infty)^k\mathbf{u}(0) + \sum_{t=0}^{k-1}(\mathbf{I} - \eta\mathbf{H}^\infty)^t\boldsymbol{\zeta}(k-1-t).\end{aligned} \tag{27}$$

Note that $\mathbf{I} - \eta\mathbf{H}^\infty$ is positive semidefinite, because we have $\left\|\mathbf{H}^\infty\right\|_2 \le \operatorname{tr}\left[\mathbf{H}^\infty\right] = \frac{n}{2}$ and $\eta = O\left(\frac{\lambda_0}{n^2}\right) = O\left(\frac{\lambda_{\min}(\mathbf{H}^\infty)}{\left\|\mathbf{H}^\infty\right\|_2^2}\right) \le \frac{1}{\left\|\mathbf{H}^\infty\right\|_2}$. This implies $\left\|\mathbf{I} - \eta\mathbf{H}^\infty\right\|_2 \le 1 - \eta\lambda_0$.

Now we study the three terms in (27) separately. The first term is exactly $\tilde{\mathbf{u}}(k) - \mathbf{y}$ (see Section 4.1), and in Section 4.1 we have shown that

$$\left\|-(\mathbf{I} - \eta\mathbf{H}^\infty)^k\mathbf{y}\right\|_2 = \sqrt{\sum_{i=1}^n(1 - \eta\lambda_i)^{2k}(\mathbf{v}_i^\top\mathbf{y})^2}. \tag{28}$$

The second term in (27) is small as long as $\mathbf{u}(0)$ is small, which is the case when the magnitude of initialization κ is set to be small. Formally, each $u_i(0)$ has zero mean and variance $O(\kappa^2)$, which means $\mathbb{E}\left[(u_i(0))^2\right] = O(\kappa^2)$. This implies $\mathbb{E}\left[\left\|\mathbf{u}(0)\right\|^2\right] = O(n\kappa^2)$, and by Markov's inequality we have $\left\|\mathbf{u}(0)\right\|^2 \le \frac{n\kappa^2}{\delta}$ with probability at least $1 - \delta$. Therefore we have

$$\left\|(\mathbf{I} - \eta\mathbf{H}^\infty)^k\mathbf{u}(0)\right\|_2 \le \left\|(\mathbf{I} - \eta\mathbf{H}^\infty)^k\right\|_2\left\|\mathbf{u}(0)\right\|_2 \le (1 - \eta\lambda_0)^k O\left(\sqrt{n}\kappa/\delta\right). \tag{29}$$

The third term in (27) can be bounded using (26). Also note that we have $\left\|\mathbf{u}(k) - \mathbf{y}\right\|_2 \le \left(1 - \frac{\eta\lambda_0}{4}\right)^k\left\|\mathbf{u}(0) - \mathbf{y}\right\|_2 =$

$\left(1-\frac{\eta\lambda_0}{4}\right)^k O(\sqrt{n/\delta})$ (Theorem 3.1). Therefore we have

$$\begin{aligned}
\left\|\sum_{t=0}^{k-1}(\mathbf{I}-\eta\mathbf{H}^\infty)^t\boldsymbol{\zeta}(k-1-t)\right\|_2 &\le \sum_{t=0}^{k-1}\|\mathbf{I}-\eta\mathbf{H}^\infty\|_2^t\,\|\boldsymbol{\zeta}(k-1-t)\|_2\\
&\le \sum_{t=0}^{k-1}(1-\eta\lambda_0)^t O\left(\frac{\eta n^3}{\sqrt{m}\lambda_0\kappa\delta^{3/2}}\right)\|\mathbf{u}(k-1-t)-\mathbf{y}\|_2\\
&\le \sum_{t=0}^{k-1}(1-\eta\lambda_0)^t O\left(\frac{\eta n^3}{\sqrt{m}\lambda_0\kappa\delta^{3/2}}\right)\left(1-\frac{\eta\lambda_0}{4}\right)^{k-1-t} O(\sqrt{n/\delta})\\
&\le k\left(1-\frac{\eta\lambda_0}{4}\right)^{k-1} O\left(\frac{\eta n^{7/2}}{\sqrt{m}\lambda_0\kappa\delta^2}\right).
\end{aligned} \tag{30}$$

Combining (27), (28), (29) and (30), we obtain

$$\begin{aligned}
\|\mathbf{u}(k)-\mathbf{y}\|_2 &= \sqrt{\sum_{i=1}^n(1-\eta\lambda_i)^{2k}(\mathbf{v}_i^\top\mathbf{y})^2} \pm O\left((1-\eta\lambda_0)^k\frac{\sqrt{n}\kappa}{\delta}+k\left(1-\frac{\eta\lambda_0}{4}\right)^{k-1}\frac{\eta n^{7/2}}{\sqrt{m}\lambda_0\kappa\delta^2}\right)\\
&= \sqrt{\sum_{i=1}^n(1-\eta\lambda_i)^{2k}(\mathbf{v}_i^\top\mathbf{y})^2} \pm O\left(\frac{\sqrt{n}\kappa}{\delta}+\frac{1}{\eta\lambda_0}\cdot\frac{\eta n^{7/2}}{\sqrt{m}\lambda_0\kappa\delta^2}\right)\\
&= \sqrt{\sum_{i=1}^n(1-\eta\lambda_i)^{2k}(\mathbf{v}_i^\top\mathbf{y})^2} \pm O\left(\frac{\sqrt{n}\kappa}{\delta}+\frac{n^{7/2}}{\sqrt{m}\lambda_0^2\kappa\delta^2}\right),
\end{aligned}$$

where we have used $\max_{k\ge0}\left\{k(1-\eta\lambda_0/4)^{k-1}\right\}=O(1/(\eta\lambda_0))$. From our choices of κ and m, the above error term is at most ϵ. This completes the proof of Theorem 4.1. □

D. Proofs for Section 5

D.1. Proof of Lemma 5.3

Proof of Lemma 5.3. We assume that all the high-probability ("with probability $1-\delta$") events happen. By a union bound at the end, the success probability is at least $1-\Omega(\delta)$, and then we can rescale δ by a constant such that the success probability is at least $1-\delta$.

The first part of Lemma 5.3 is proved as Lemma C.1 (note that $\|\mathbf{y}-\mathbf{u}(0)\|_2=O\left(\sqrt{n/\delta}\right)$). Now we prove the second part.

Recall the update rule (6) for $\mathbf{W}$:

$$\operatorname{vec}(\mathbf{W}(k+1))=\operatorname{vec}(\mathbf{W}(k))-\eta\mathbf{Z}(k)(\mathbf{u}(k)-\mathbf{y}). \tag{31}$$

According to the proof of Theorem 4.1 ((27), (29) and (30)) we can write

$$\mathbf{u}(k)-\mathbf{y}=-(\mathbf{I}-\eta\mathbf{H}^\infty)^k\mathbf{y}+\mathbf{e}(k), \tag{32}$$

where

$$\|\mathbf{e}(k)\|=O\left((1-\eta\lambda_0)^k\cdot\frac{\sqrt{n}\kappa}{\delta}+k\left(1-\frac{\eta\lambda_0}{4}\right)^{k-1}\cdot\frac{\eta n^{7/2}}{\sqrt{m}\lambda_0\kappa\delta^2}\right). \tag{33}$$

Plugging (32) into (31) and taking a sum over $k = 0, 1, \ldots, K-1$, we get:

$$
\begin{aligned}
&\operatorname{vec}(\mathbf{W}(K)) - \operatorname{vec}(\mathbf{W}(0)) \\
=& \sum_{k=0}^{K-1} \left(\operatorname{vec}(\mathbf{W}(k+1)) - \operatorname{vec}(\mathbf{W}(k))\right) \\
=& -\sum_{k=0}^{K-1} \eta \mathbf{Z}(k)(\mathbf{u}(k) - \mathbf{y}) \\
=& \sum_{k=0}^{K-1} \eta \mathbf{Z}(k) \left((\mathbf{I} - \eta \mathbf{H}^{\infty})^k \mathbf{y} - \mathbf{e}(k)\right) \\
=& \sum_{k=0}^{K-1} \eta \mathbf{Z}(k)(\mathbf{I} - \eta \mathbf{H}^{\infty})^k \mathbf{y} - \sum_{k=0}^{K-1} \eta \mathbf{Z}(k)\mathbf{e}(k) \\
=& \sum_{k=0}^{K-1} \eta \mathbf{Z}(0)(\mathbf{I} - \eta \mathbf{H}^{\infty})^k \mathbf{y} + \sum_{k=0}^{K-1} \eta (\mathbf{Z}(k) - \mathbf{Z}(0))(\mathbf{I} - \eta \mathbf{H}^{\infty})^k \mathbf{y} - \sum_{k=0}^{K-1} \eta \mathbf{Z}(k)\mathbf{e}(k).
\end{aligned}
\tag{34}
$$

The second and the third terms in (34) are considered perturbations, and we can upper bound their norms easily. For the second term, using $\left\|\mathbf{Z}(k) - \mathbf{Z}(0)\right\|_F = O\left(\frac{n}{\sqrt{m^{1/2}\lambda_0\kappa\delta^{3/2}}}\right)$ (Lemma C.2), we have:

$$
\begin{aligned}
&\left\| \sum_{k=0}^{K-1} \eta (\mathbf{Z}(k) - \mathbf{Z}(0))(\mathbf{I} - \eta \mathbf{H}^{\infty})^k \mathbf{y} \right\|_2 \\
\leq& \sum_{k=0}^{K-1} \eta \cdot O\left(\frac{n}{\sqrt{m^{1/2}\lambda_0\kappa\delta^{3/2}}}\right) \left\|\mathbf{I} - \eta \mathbf{H}^{\infty}\right\|_2^k \left\|\mathbf{y}\right\|_2 \\
\leq& O\left(\frac{\eta n}{\sqrt{m^{1/2}\lambda_0\kappa\delta^{3/2}}}\right) \sum_{k=0}^{K-1} (1 - \eta\lambda_0)^k \sqrt{n} \\
=& O\left(\frac{n^{3/2}}{\sqrt{m^{1/2}\lambda_0^3\kappa\delta^{3/2}}}\right).
\end{aligned}
\tag{35}
$$

For the third term in (34), we use $\left\|\mathbf{Z}(k)\right\|_F \leq \sqrt{n}$ and (33) to get:

$$
\begin{aligned}
&\left\| \sum_{k=0}^{K-1} \eta \mathbf{Z}(k)\mathbf{e}(k) \right\|_2 \\
\leq& \sum_{k=0}^{K-1} \eta \sqrt{n} \cdot O\left((1 - \eta\lambda_0)^k \cdot \frac{\sqrt{n}\kappa}{\delta} + k\left(1 - \frac{\eta\lambda_0}{4}\right)^{k-1} \cdot \frac{\eta n^{7/2}}{\sqrt{m}\lambda_0\kappa\delta^2} \right) \\
=& O\left(\frac{\eta n \kappa}{\delta} \sum_{k=0}^{K-1} (1 - \eta\lambda_0)^k + \frac{\eta^2 n^4}{\sqrt{m}\lambda_0\kappa\delta^2} \sum_{k=0}^{K-1} k\left(1 - \frac{\eta\lambda_0}{4}\right)^{k-1} \right) \\
=& O\left(\frac{n\kappa}{\lambda_0\delta} + \frac{n^4}{\sqrt{m}\lambda_0^3\kappa\delta^2} \right).
\end{aligned}
\tag{36}
$$

Define $\mathbf{T} = \eta \sum_{k=0}^{K-1} (\mathbf{I} - \eta \mathbf{H}^{\infty})^k$. For the first term in (34), using $\left\|\mathbf{H}(0) - \mathbf{H}^{\infty}\right\|_F = O\left(\frac{n\sqrt{\log\frac{n}{\delta}}}{\sqrt{m}}\right)$ (Lemma C.3) we have

$$\begin{aligned}
&\left\|\sum_{k=0}^{K-1}\eta\mathbf{Z}(0)(\mathbf{I}-\eta\mathbf{H}^\infty)^k\mathbf{y}\right\|_2^2\\
=&\ \|\mathbf{Z}(0)\mathbf{T}\mathbf{y}\|_2^2\\
=&\,\mathbf{y}^\top\mathbf{T}\mathbf{Z}(0)^\top\mathbf{Z}(0)\mathbf{T}\mathbf{y}\\
=&\,\mathbf{y}^\top\mathbf{T}\mathbf{H}(0)\mathbf{T}\mathbf{y}\\
\le&\,\mathbf{y}^\top\mathbf{T}\mathbf{H}^\infty\mathbf{T}\mathbf{y}+\|\mathbf{H}(0)-\mathbf{H}^\infty\|_2\,\|\mathbf{T}\|_2^2\,\|\mathbf{y}\|_2^2\\
\le&\,\mathbf{y}^\top\mathbf{T}\mathbf{H}^\infty\mathbf{T}\mathbf{y}+O\left(\frac{n\sqrt{\log\frac{n}{\delta}}}{\sqrt{m}}\right)\cdot\left(\eta\sum_{k=0}^{K-1}(\mathbf{I}-\eta\lambda_0)^k\right)^2 n\\
=&\,\mathbf{y}^\top\mathbf{T}\mathbf{H}^\infty\mathbf{T}\mathbf{y}+O\left(\frac{n^2\sqrt{\log\frac{n}{\delta}}}{\sqrt{m}\lambda_0^2}\right).
\end{aligned}\tag{37}$$

Let the eigen-decomposition of $\mathbf{H}^\infty$ be $\mathbf{H}^\infty=\sum_{i=1}^n\lambda_i\mathbf{v}_i\mathbf{v}_i^\top$. Since $\mathbf{T}$ is a polynomial of $\mathbf{H}^\infty$, it has the same set of eigenvectors as $\mathbf{H}^\infty$, and we have

$$\mathbf{T}=\sum_{i=1}^n\eta\sum_{k=0}^{K-1}(1-\eta\lambda_i)^k\mathbf{v}_i\mathbf{v}_i^\top=\sum_{i=1}^n\frac{1-(1-\eta\lambda_i)^K}{\lambda_i}\mathbf{v}_i\mathbf{v}_i^\top.$$

It follows that

$$\mathbf{T}\mathbf{H}^\infty\mathbf{T}=\sum_{i=1}^n\left(\frac{1-(1-\eta\lambda_i)^K}{\lambda_i}\right)^2\lambda_i\mathbf{v}_i\mathbf{v}_i^\top\preceq\sum_{i=1}^n\frac{1}{\lambda_i}\mathbf{v}_i\mathbf{v}_i^\top=(\mathbf{H}^\infty)^{-1}.$$

Plugging this into (37), we get

$$\left\|\sum_{k=0}^{K-1}\eta\mathbf{Z}(0)(\mathbf{I}-\eta\mathbf{H}^\infty)^k\mathbf{y}\right\|_2\le\sqrt{\mathbf{y}^\top(\mathbf{H}^\infty)^{-1}\mathbf{y}+O\left(\frac{n^2\sqrt{\log\frac{n}{\delta}}}{\sqrt{m}\lambda_0^2}\right)}\le\sqrt{\mathbf{y}^\top(\mathbf{H}^\infty)^{-1}\mathbf{y}}+O\left(\sqrt{\frac{n^2\sqrt{\log\frac{n}{\delta}}}{\sqrt{m}\lambda_0^2}}\right).\tag{38}$$

Finally, plugging the three bounds (35), (36) and (38) into (34), we have

$$\begin{aligned}
&\|\mathbf{W}(K)-\mathbf{W}(0)\|_F\\
=&\ \|\mathrm{vec}\,(\mathbf{W}(K))-\mathrm{vec}\,(\mathbf{W}(0))\|_2\\
\le&\sqrt{\mathbf{y}^\top(\mathbf{H}^\infty)^{-1}\mathbf{y}}+O\left(\sqrt{\frac{n^2\sqrt{\log\frac{n}{\delta}}}{\sqrt{m}\lambda_0^2}}\right)+O\left(\frac{n^{3/2}}{\sqrt{m^{1/2}\lambda_0^3\kappa\delta^{3/2}}}\right)+O\left(\frac{n\kappa}{\lambda_0\delta}+\frac{n^4}{\sqrt{m}\lambda_0^3\kappa\delta^2}\right)\\
=&\sqrt{\mathbf{y}^\top(\mathbf{H}^\infty)^{-1}\mathbf{y}}+O\left(\frac{n\kappa}{\lambda_0\delta}\right)+\frac{\mathrm{poly}\left(n,\frac{1}{\lambda_0},\frac{1}{\delta}\right)}{m^{1/4}\kappa^{1/2}}.
\end{aligned}$$

This finishes the proof of Lemma 5.3. □

D.2. Proof of Lemma 5.4

Proof of Lemma 5.4. We need to upper bound

$$\begin{aligned}
\mathcal{R}_S\left(\mathcal{F}_{R,B}^{\mathbf{W}(0),\mathbf{a}}\right)&=\frac{1}{n}\mathop{\mathbb{E}}_{\boldsymbol{\varepsilon}\sim\{\pm1\}^n}\left[\sup_{f\in\mathcal{F}_{R,B}^{\mathbf{W}(0),\mathbf{a}}}\sum_{i=1}^n\varepsilon_i f(\mathbf{x}_i)\right]\\
&=\frac{1}{n}\mathop{\mathbb{E}}_{\boldsymbol{\varepsilon}\sim\{\pm1\}^n}\left[\sup_{\substack{\mathbf{W}:\|\mathbf{W}-\mathbf{W}(0)\|_{2,\infty}\le R\\\|\mathbf{W}-\mathbf{W}(0)\|_F\le B}}\sum_{i=1}^n\varepsilon_i f_{\mathbf{W},\mathbf{a}}(\mathbf{x}_i)\right]
\end{aligned}$$

$$= \frac{1}{n} \mathop{\mathbb{E}}_{\boldsymbol{\varepsilon}\sim\{\pm1\}^n} \left[\sup_{\substack{\mathbf{W}: \|\mathbf{W}-\mathbf{W}(0)\|_{2,\infty}\le R \\ \|\mathbf{W}-\mathbf{W}(0)\|_F \le B}} \sum_{i=1}^n \varepsilon_i \sum_{r=1}^m \frac{1}{\sqrt{m}} a_r \sigma(\mathbf{w}^\top \mathbf{x}_i) \right],$$

where $\|\mathbf{W}-\mathbf{W}(0)\|_{2,\infty} = \max_{r\in[m]} \|\mathbf{w}_r - \mathbf{w}_r(0)\|_2$.

Similar to the proof of Lemma C.2, we define events:

$$A_{r,i} = \left\{ \left|\mathbf{w}_r(0)^\top \mathbf{x}_i\right| \le R \right\}, \quad i \in [n], r \in [m].$$

Since we only look at $\mathbf{W}$ such that $\|\mathbf{w}_r - \mathbf{w}_r(0)\|_2 \le R$ for all $r \in [m]$, if $\mathbb{I}\{A_{r,i}\} = 0$ we must have $\mathbb{I}\{\mathbf{w}^\top \mathbf{x}_i\} = \mathbb{I}\{\mathbf{w}_r(0)^\top \mathbf{x}_i \ge 0\} = \mathbb{I}_{r,i}(0)$. Thus we have

$$\mathbb{I}\left\{\neg A_{r,i}\right\} \sigma\left(\mathbf{w}_r^\top \mathbf{x}_i\right) = \mathbb{I}\left\{\neg A_{r,i}\right\} \mathbb{I}_{r,i}(0) \mathbf{w}_r^\top \mathbf{x}_i.$$

Then we have

$$\begin{aligned}
&\sum_{i=1}^n \varepsilon_i \sum_{r=1}^m a_r \sigma\left(\mathbf{w}_r^\top \mathbf{x}_i\right) - \sum_{i=1}^n \varepsilon_i \sum_{r=1}^m a_r \mathbb{I}_{r,i}(0) \mathbf{w}_r^\top \mathbf{x}_i \\
=& \sum_{r=1}^m \sum_{i=1}^n \left(\mathbb{I}\left\{A_{r,i}\right\} + \mathbb{I}\left\{\neg A_{r,i}\right\}\right) \varepsilon_i a_r \left(\sigma\left(\mathbf{w}_r^\top \mathbf{x}_i\right) - \mathbb{I}_{r,i}(0)\mathbf{w}_r^\top \mathbf{x}_i\right) \\
=& \sum_{r=1}^m \sum_{i=1}^n \mathbb{I}\left\{A_{r,i}\right\} \varepsilon_i a_r \left(\sigma\left(\mathbf{w}_r^\top \mathbf{x}_i\right) - \mathbb{I}_{r,i}(0)\mathbf{w}_r^\top \mathbf{x}_i\right) \\
=& \sum_{r=1}^m \sum_{i=1}^n \mathbb{I}\left\{A_{r,i}\right\} \varepsilon_i a_r \left(\sigma\left(\mathbf{w}_r^\top \mathbf{x}_i\right) - \mathbb{I}_{r,i}(0)\mathbf{w}_r(0)^\top \mathbf{x}_i - \mathbb{I}_{r,i}(0)(\mathbf{w}_r - \mathbf{w}_r(0))^\top \mathbf{x}_i\right) \\
=& \sum_{r=1}^m \sum_{i=1}^n \mathbb{I}\left\{A_{r,i}\right\} \varepsilon_i a_r \left(\sigma\left(\mathbf{w}_r^\top \mathbf{x}_i\right) - \sigma\left(\mathbf{w}_r(0)^\top \mathbf{x}_i\right) - \mathbb{I}_{r,i}(0)(\mathbf{w}_r - \mathbf{w}_r(0))^\top \mathbf{x}_i\right) \\
\le& \sum_{r=1}^m \sum_{i=1}^n \mathbb{I}\left\{A_{r,i}\right\} \cdot 2R.
\end{aligned}$$

Thus we can bound the Rademacher complexity as:

$$\begin{aligned}
\mathcal{R}_S\left(\mathcal{F}_{R,B}^{\mathbf{W}(0),\mathbf{a}}\right) &= \frac{1}{n} \mathop{\mathbb{E}}_{\boldsymbol{\varepsilon}\sim\{\pm1\}^n} \left[\sup_{\substack{\mathbf{W}: \|\mathbf{W}-\mathbf{W}(0)\|_{2,\infty}\le R \\ \|\mathbf{W}-\mathbf{W}(0)\|_F \le B}} \sum_{i=1}^n \varepsilon_i \sum_{r=1}^m \frac{a_r}{\sqrt{m}} \sigma\left(\mathbf{w}_r^\top \mathbf{x}\right) \right] \\
&\le \frac{1}{n} \mathop{\mathbb{E}}_{\boldsymbol{\varepsilon}\sim\{\pm1\}^n} \left[\sup_{\substack{\mathbf{W}: \|\mathbf{W}-\mathbf{W}(0)\|_{2,\infty}\le R \\ \|\mathbf{W}-\mathbf{W}(0)\|_F \le B}} \sum_{i=1}^n \varepsilon_i \sum_{r=1}^m \frac{a_r}{\sqrt{m}} \mathbb{I}_{r,i}(0) \mathbf{w}_r^\top \mathbf{x}_i \right] + \frac{2R}{n\sqrt{m}} \sum_{r=1}^m \sum_{i=1}^n \mathbb{I}\left\{A_{r,i}\right\} \\
&\le \frac{1}{n} \mathop{\mathbb{E}}_{\boldsymbol{\varepsilon}\sim\{\pm1\}^n} \left[\sup_{\mathbf{W}: \|\mathbf{W}-\mathbf{W}(0)\|_F \le B} \sum_{i=1}^n \varepsilon_i \sum_{r=1}^m \frac{a_r}{\sqrt{m}} \mathbb{I}_{r,i}(0) \mathbf{w}_r^\top \mathbf{x}_i \right] + \frac{2R}{n\sqrt{m}} \sum_{r=1}^m \sum_{i=1}^n \mathbb{I}\left\{A_{r,i}\right\} \\
&= \frac{1}{n} \mathop{\mathbb{E}}_{\boldsymbol{\varepsilon}\sim\{\pm1\}^n} \left[\sup_{\mathbf{W}: \|\mathbf{W}-\mathbf{W}(0)\|_F \le B} \mathrm{vec}\left(\mathbf{W}\right)^\top \mathbf{Z}(0) \boldsymbol{\varepsilon} \right] + \frac{2R}{n\sqrt{m}} \sum_{r=1}^m \sum_{i=1}^n \mathbb{I}\left\{A_{r,i}\right\} \\
&= \frac{1}{n} \mathop{\mathbb{E}}_{\boldsymbol{\varepsilon}\sim\{\pm1\}^n} \left[\sup_{\mathbf{W}: \|\mathbf{W}-\mathbf{W}(0)\|_F \le B} \mathrm{vec}\left(\mathbf{W}-\mathbf{W}(0)\right)^\top \mathbf{Z}(0) \boldsymbol{\varepsilon} \right] + \frac{2R}{n\sqrt{m}} \sum_{r=1}^m \sum_{i=1}^n \mathbb{I}\left\{A_{r,i}\right\} \\
&\le \frac{1}{n} \mathop{\mathbb{E}}_{\boldsymbol{\varepsilon}\sim\{\pm1\}^n} \left[B \cdot \|\mathbf{Z}(0)\boldsymbol{\varepsilon}\|_2 \right] + \frac{2R}{n\sqrt{m}} \sum_{r=1}^m \sum_{i=1}^n \mathbb{I}\left\{A_{r,i}\right\}
\end{aligned}$$

$$
\begin{aligned}
&\leq \frac{B}{n}\sqrt{\mathop{\mathbb{E}}_{\boldsymbol{\varepsilon}\sim\{\pm 1\}^n}\left[\left\|\mathbf{Z}(0)\boldsymbol{\varepsilon}\right\|_2^2\right]} + \frac{2R}{n\sqrt{m}}\sum_{r=1}^{m}\sum_{i=1}^{n}\mathbb{I}\left\{A_{r,i}\right\}\\
&= \frac{B}{n}\left\|\mathbf{Z}(0)\right\|_F + \frac{2R}{n\sqrt{m}}\sum_{r=1}^{m}\sum_{i=1}^{n}\mathbb{I}\left\{A_{r,i}\right\}.
\end{aligned}
$$

Next we bound $\left\|\mathbf{Z}(0)\right\|_F$ and $\sum_{r=1}^{m}\sum_{i=1}^{n}\mathbb{I}\left\{A_{r,i}\right\}$.

For $\left\|\mathbf{Z}(0)\right\|_F$, notice that

$$
\left\|\mathbf{Z}(0)\right\|_F^2 = \frac{1}{m}\sum_{r=1}^{m}\left(\sum_{i=1}^{n}\mathbb{I}_{r,i}(0)\right).
$$

Since all m neurons are independent at initialization and $\mathbb{E}\left[\sum_{i=1}^{n}\mathbb{I}_{r,i}(0)\right] = n/2$, by Hoeffding's inequality, with probability at least $1-\delta/2$ we have

$$
\left\|\mathbf{Z}(0)\right\|_F^2 \leq n\left(\frac{1}{2} + \sqrt{\frac{\log\frac{2}{\delta}}{2m}}\right).
$$

Similarly, for $\sum_{r=1}^{m}\sum_{i=1}^{n}\mathbb{I}\left\{A_{r,i}\right\}$, from (17) we know $\mathbb{E}\left[\sum_{i=1}^{n}\mathbb{I}\left\{A_{r,i}\right\}\right] \leq \frac{\sqrt{2}nR}{\sqrt{\pi}\kappa}$. Then by Hoeffding's inequality, with probability at least $1-\delta/2$ we have

$$
\sum_{r=1}^{m}\sum_{i=1}^{n}\mathbb{I}\left\{A_{r,i}\right\} \leq mn\left(\frac{\sqrt{2}R}{\sqrt{\pi}\kappa} + \sqrt{\frac{\log\frac{2}{\delta}}{2m}}\right).
$$

Therefore, with probability at least $1-\delta$, the Rademacher complexity is bounded as:

$$
\begin{aligned}
\mathcal{R}_S\left(\mathcal{F}_{R,B}^{\mathbf{W}(0),\mathbf{a}}\right) &\leq \frac{B}{n}\left(\sqrt{\frac{n}{2}} + \sqrt{n\sqrt{\frac{\log\frac{2}{\delta}}{2m}}}\right) + \frac{2R}{n\sqrt{m}}mn\left(\frac{\sqrt{2}R}{\sqrt{\pi}\kappa} + \sqrt{\frac{\log\frac{2}{\delta}}{2m}}\right)\\
&= \frac{B}{\sqrt{2n}}\left(1 + \left(\frac{2\log\frac{2}{\delta}}{m}\right)^{1/4}\right) + \frac{2\sqrt{2}R^2\sqrt{m}}{\sqrt{\pi}\kappa} + R\sqrt{2\log\frac{2}{\delta}},
\end{aligned}
$$

completing the proof of Lemma 5.4. (Note that the high probability events used in the proof do not depend on the value of B, so the above bound holds simultaneously for every B.) □

D.3. Proof of Theorem 5.1

Proof of Theorem 5.1. First of all, since the distribution $\mathcal{D}$ is $(\lambda_0, \delta/3, n)$-non-degenerate, with probability at least $1-\delta/3$ we have $\lambda_{\min}(\mathbf{H}^\infty) \geq \lambda_0$. The rest of the proof is conditioned on this happening.

Next, from Theorem 3.1, Lemma 5.3 and Lemma 5.4, we know that for any sample S, with probability at least $1-\delta/3$ over the random initialization, the followings hold simultaneously:

(i) Optimization succeeds (Theorem 3.1):

$$
\Phi(\mathbf{W}(k)) \leq \left(1 - \frac{\eta\lambda_0}{2}\right)^k \cdot O\left(\frac{n}{\delta}\right) \leq \frac{1}{2}.
$$

This implies an upper bound on the training error $L_S(f_{\mathbf{W}(k),\mathbf{a}}) = \frac{1}{n}\sum_{i=1}^{n}\ell(f_{\mathbf{W}(k),\mathbf{a}}(\mathbf{x}_i), y_i) = \frac{1}{n}\sum_{i=1}^{n}\ell(u_i(k), y_i)$:

$$
L_S(f_{\mathbf{W}(k),\mathbf{a}}) = \frac{1}{n}\sum_{i=1}^{n}\left[\ell(u_i(k), y_i) - \ell(y_i, y_i)\right]
$$

$$
\begin{aligned}
&\le \frac{1}{n}\sum_{i=1}^{n}\left|u_i(k)-y_i\right| \\
&\le \frac{1}{\sqrt{n}}\left\|\mathbf{u}(k)-\mathbf{y}\right\|_2 \\
&= \sqrt{\frac{2\Phi(\mathbf{W}(k))}{n}} \\
&\le \frac{1}{\sqrt{n}}.
\end{aligned}
$$

(ii) $\left\|\mathbf{w}_r(k)-\mathbf{w}_r(0)\right\|_2 \le R$ ($\forall r \in [m]$) and $\left\|\mathbf{W}(k)-\mathbf{W}(0)\right\|_F \le B$, where $R = O\left(\frac{n}{\sqrt{m}\lambda_0\sqrt{\delta}}\right)$ and $B = \sqrt{\mathbf{y}^\top\left(\mathbf{H}^\infty\right)^{-1}\mathbf{y}} + O\left(\frac{n\kappa}{\lambda_0\delta}\right) + \frac{\mathrm{poly}\left(n,\lambda_0^{-1},\delta^{-1}\right)}{m^{1/4}\kappa^{1/2}}$. Note that $B \le O\left(\sqrt{\frac{n}{\lambda_0}}\right)$.

(iii) Let $B_i = i$ ($i = 1, 2, \ldots$). Simultaneously for all i, the function class $\mathcal{F}_{R,B_i}^{\mathbf{W}(0),\mathbf{a}}$ has Rademacher complexity bounded as

$$
\mathcal{R}_S\left(\mathcal{F}_{R,B_i}^{\mathbf{W}(0),\mathbf{a}}\right) \le \frac{B_i}{\sqrt{2n}}\left(1+\left(\frac{2\log\frac{10}{\delta}}{m}\right)^{1/4}\right) + \frac{2R^2\sqrt{m}}{\kappa} + R\sqrt{2\log\frac{10}{\delta}}.
$$

Let i^* be the smallest integer such that $B \le B_{i^*}$. Then we have $i^* \le O\left(\sqrt{\frac{n}{\lambda_0}}\right)$ and $B_{i^*} \le B+1$. From above we know $f_{\mathbf{W}(k),\mathbf{a}} \in \mathcal{F}_{R,B_{i^*}}^{\mathbf{W}(0),\mathbf{a}}$, and

$$
\begin{aligned}
&\mathcal{R}_S\left(\mathcal{F}_{R,B_{i^*}}^{\mathbf{W}(0),\mathbf{a}}\right) \\
\le\, & \frac{B+1}{\sqrt{2n}}\left(1+\left(\frac{2\log\frac{10}{\delta}}{m}\right)^{1/4}\right) + \frac{2R^2\sqrt{m}}{\kappa} + R\sqrt{2\log\frac{10}{\delta}} \\
=\, & \frac{\sqrt{\mathbf{y}^\top\left(\mathbf{H}^\infty\right)^{-1}\mathbf{y}}}{\sqrt{2n}}\left(1+\left(\frac{2\log\frac{10}{\delta}}{m}\right)^{1/4}\right) + \frac{1}{\sqrt{n}} + O\left(\frac{\sqrt{n}\kappa}{\lambda_0\delta}\right) + \frac{\mathrm{poly}\left(n,\lambda_0^{-1},\delta^{-1}\right)}{m^{1/4}\kappa^{1/2}} + \frac{2R^2\sqrt{m}}{\kappa} + R\sqrt{2\log\frac{10}{\delta}} \\
\le\, & \sqrt{\frac{\mathbf{y}^\top\left(\mathbf{H}^\infty\right)^{-1}\mathbf{y}}{2n}} + \sqrt{\frac{\sqrt{n}\lambda_0^{-1}\sqrt{n}}{2n}}\left(\frac{2\log\frac{10}{\delta}}{m}\right)^{1/4} + \frac{1}{\sqrt{n}} + O\left(\frac{\sqrt{n}\kappa}{\lambda_0\delta}\right) + \frac{\mathrm{poly}\left(n,\lambda_0^{-1},\delta^{-1}\right)}{m^{1/4}\kappa^{1/2}} \\
=\, & \sqrt{\frac{\mathbf{y}^\top\left(\mathbf{H}^\infty\right)^{-1}\mathbf{y}}{2n}} + \frac{1}{\sqrt{n}} + O\left(\frac{\sqrt{n}\kappa}{\lambda_0\delta}\right) + \frac{\mathrm{poly}\left(n,\lambda_0^{-1},\delta^{-1}\right)}{m^{1/4}\kappa^{1/2}} \\
\le\, & \sqrt{\frac{\mathbf{y}^\top\left(\mathbf{H}^\infty\right)^{-1}\mathbf{y}}{2n}} + \frac{2}{\sqrt{n}}.
\end{aligned}
$$

Next, from the theory of Rademacher complexity (Theorem B.1) and a union bound over a finite set of different i's, for any random initialization $(\mathbf{W}(0), \mathbf{a})$, with probability at least $1-\delta/3$ over the sample S, we have

$$
\sup_{f\in\mathcal{F}_{R,B_i}^{\mathbf{W}(0),\mathbf{a}}}\left\{L_{\mathcal{D}}(f)-L_S(f)\right\} \le 2\mathcal{R}_S\left(\mathcal{F}_{R,B_i}^{\mathbf{W}(0),\mathbf{a}}\right) + O\left(\sqrt{\frac{\log\frac{n}{\lambda_0\delta}}{n}}\right), \qquad \forall i \in \left\{1, 2, \ldots, O\left(\sqrt{\frac{n}{\lambda_0}}\right)\right\}.
$$

Finally, taking a union bound, we know that with probability at least $1-\frac{2}{3}\delta$ over the sample S and the random initialization

$(\mathbf{W}(0), \mathbf{a})$, the followings are all satisfied (for some i^*):

$$L_S(f_{\mathbf{W}(k),\mathbf{a}}) \le \frac{1}{\sqrt{n}},$$
$$f_{\mathbf{W}(k),\mathbf{a}} \in \mathcal{F}^{\mathbf{W}(0),\mathbf{a}}_{R,B_{i^*}},$$
$$\mathcal{R}_S\left(\mathcal{F}^{\mathbf{W}(0),\mathbf{a}}_{R,B_{i^*}}\right) \le \sqrt{\frac{\mathbf{y}^\top \left(\mathbf{H}^\infty\right)^{-1}\mathbf{y}}{2n}} + \frac{2}{\sqrt{n}},$$
$$\sup_{f\in\mathcal{F}^{\mathbf{W}(0),\mathbf{a}}_{R,B_{i^*}}} \{L_\mathcal{D}(f) - L_S(f)\} \le 2\mathcal{R}_S\left(\mathcal{F}^{\mathbf{W}(0),\mathbf{a}}_{R,B_{i^*}}\right) + O\left(\sqrt{\frac{\log\frac{n}{\lambda_0\delta}}{n}}\right).$$

These together can imply:

$$\begin{aligned}
L_\mathcal{D}(f_{\mathbf{W}(k),\mathbf{a}}) &\le \frac{1}{\sqrt{n}} + 2\mathcal{R}_S\left(\mathcal{F}^{\mathbf{W}(0),\mathbf{a}}_{R,B_{i^*}}\right) + O\left(\sqrt{\frac{\log\frac{n}{\lambda_0\delta}}{n}}\right) \\
&\le \frac{1}{\sqrt{n}} + 2\left(\sqrt{\frac{\mathbf{y}^\top \left(\mathbf{H}^\infty\right)^{-1}\mathbf{y}}{2n}} + \frac{2}{\sqrt{n}}\right) + O\left(\sqrt{\frac{\log\frac{n}{\lambda_0\delta}}{n}}\right) \\
&= \sqrt{\frac{2\mathbf{y}^\top \left(\mathbf{H}^\infty\right)^{-1}\mathbf{y}}{n}} + O\left(\sqrt{\frac{\log\frac{n}{\lambda_0\delta}}{n}}\right).
\end{aligned}$$

This completes the proof. □

D.4. Proof of Corollary 5.2

Proof of Corollary 5.2. We apply Theorem 5.1 to the ramp loss

$$\ell^{\text{ramp}}(u,y) = \begin{cases} 1, & uy \le 0, \\ 1-uy, & 0 < uy < 1, \\ 0, & uy \ge 1. \end{cases} \qquad (u\in\mathbb{R}, y\in\{\pm 1\})$$

Note that it is 1-Lipschitz in u for $y \in \{\pm 1\}$ and satisfies $\ell^{\text{ramp}}(y,y) = 0$ for $y \in \{\pm 1\}$. It is also an upper bound on the 0-1 loss:

$$\ell^{\text{ramp}}(u,y) \ge \ell^{01}(u,y) = \mathbb{I}\left\{uy \le 0\right\}.$$

Therefore we have with probability at least $1-\delta$:

$$\begin{aligned}
L^{01}_\mathcal{D}(f_{\mathbf{W}(k),\mathbf{a}}) &= \mathop{\mathbb{E}}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell^{01}(f_{\mathbf{W}(k),\mathbf{a}}(\mathbf{x}), y)\right] \\
&\le \mathop{\mathbb{E}}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell^{\text{ramp}}(f_{\mathbf{W}(k),\mathbf{a}}(\mathbf{x}), y)\right] \\
&\le \sqrt{\frac{2\mathbf{y}^\top(\mathbf{H}^\infty)^{-1}\mathbf{y}}{n}} + O\left(\sqrt{\frac{\log\frac{n}{\lambda_0\delta}}{n}}\right).
\end{aligned}$$
□

E. Proofs for Section 6

We prove a lemma before proving Theorem 6.1.

Lemma E.1. *For any two symmetric matrices $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{n\times n}$ such that $\mathbf{B} \succeq \mathbf{A} \succeq \mathbf{0}$, we have $\mathbf{A}^\dagger \succeq \mathbf{P}_\mathbf{A}\mathbf{B}^\dagger\mathbf{P}_\mathbf{A}$, where $\mathbf{P}_\mathbf{A} = \mathbf{A}^{1/2}\mathbf{A}^\dagger\mathbf{A}^{1/2}$ is the projection matrix for the subspace spanned by $\mathbf{A}$.*[6]

Note that when $\mathbf{A}$ and $\mathbf{B}$ are both invertible, this result reads $\mathbf{A}^{-1} \succeq \mathbf{B}^{-1}$.

[6] $\mathbf{A}^\dagger$ is the Moore-Penrose pseudo-inverse of $\mathbf{A}$.

Proof. W.L.O.G. we can assume $\mathbf{B}$ is invertible, which means $\mathbf{B}^{-1} = \mathbf{B}^\dagger$. Additionally, we can assume $\mathbf{A}$ is diagonal and $\mathbf{A} = \begin{pmatrix} \mathbf{\Lambda} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$. Thus $\mathbf{P}_\mathbf{A} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$. We define $\mathbf{P}_\mathbf{A}^\perp = \mathbf{I} - \mathbf{P}_\mathbf{A} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$.

Now we will show that all the solutions to the equation $\det(\mathbf{P}_\mathbf{A}\mathbf{B}^{-1}\mathbf{P}_\mathbf{A} - \lambda(\mathbf{A}^\dagger + \mathbf{P}_\mathbf{A}^\perp)) = 0$ are between 0 and 1. If this is shown, we must have $\mathbf{P}_\mathbf{A}\mathbf{B}^{-1}\mathbf{P}_\mathbf{A} \preceq \mathbf{A}^\dagger + \mathbf{P}_\mathbf{A}^\perp$, which would imply $\mathbf{P}_\mathbf{A}\mathbf{B}^{-1}\mathbf{P}_\mathbf{A} \preceq \mathbf{A}^\dagger$.

We have

$$\begin{aligned}
&\det(\mathbf{P}_\mathbf{A}\mathbf{B}^{-1}\mathbf{P}_\mathbf{A} - \lambda(\mathbf{A}^\dagger + \mathbf{P}_\mathbf{A}^\perp)) \\
=&\det(\mathbf{B}^{-1}\mathbf{P}_\mathbf{A} - \lambda(\mathbf{A}^\dagger + \mathbf{P}_\mathbf{A}^\perp)) \\
=&\det(\mathbf{B}^{-1})\det(\mathbf{P}_\mathbf{A} - \lambda\mathbf{B}(\mathbf{A}^\dagger + \mathbf{P}_\mathbf{A}^\perp)) \\
=&\det(\mathbf{B}^{-1})\det((\mathbf{A} - \lambda\mathbf{B})(\mathbf{A}^\dagger + \mathbf{P}_\mathbf{A}^\perp)) \\
=&\det(\mathbf{B}^{-1})\det(\mathbf{A}^\dagger + \mathbf{P}_\mathbf{A}^\perp)\det(\mathbf{A} - \lambda\mathbf{B}).
\end{aligned} \tag{39}$$

Note $\det(\mathbf{B}^{-1}) > 0$ and $\det(\mathbf{A}^\dagger + \mathbf{P}_\mathbf{A}^\perp) > 0$. Thus all the solutions to $\det(\mathbf{P}_\mathbf{A}\mathbf{B}^{-1}\mathbf{P}_\mathbf{A} - \lambda(\mathbf{A}^\dagger + \mathbf{P}_\mathbf{A}^\perp)) = 0$ are exactly all the solutions to $\det(\mathbf{A} - \lambda\mathbf{B}) = 0$. Since $\mathbf{B} \succeq \mathbf{A} \succeq \mathbf{0}$ and $\mathbf{B} \succ \mathbf{0}$, we have $\det(\mathbf{A} - \lambda\mathbf{B}) \neq 0$ when $\lambda < 0$ or $\lambda > 1$. □

Proof of Theorem 6.1. For vectors $\mathbf{a} = (a_1, \ldots, a_{n_1})^\top \in \mathbb{R}^{n_1}, \mathbf{b} = (b_1, \ldots, b_{n_2}) \in \mathbb{R}^{n_2}$, the *tensor product* of $\mathbf{a}$ and $\mathbf{b}$ is defined as $\mathbf{a} \otimes \mathbf{b} \in \mathbb{R}^{n_1 n_2}$, where $[\mathbf{a} \otimes \mathbf{b}]_{(i-1)n_2+j} = a_i b_j$. For matrices $\mathbf{A} = (\mathbf{a}_1, \ldots, \mathbf{a}_{n_3}) \in \mathbb{R}^{n_1 \times n_3}, \mathbf{B} = (\mathbf{b}_1, \ldots, \mathbf{b}_{n_3}) \in \mathbb{R}^{n_2 \times n_3}$, the *Khatri-Rao product* of $\mathbf{A}$ and $\mathbf{B}$ is defined as $\mathbf{A} \odot \mathbf{B} \in \mathbb{R}^{n_1 n_2 \times n_3}$, where $\mathbf{A} \odot \mathbf{B} = [\mathbf{a}_1 \otimes \mathbf{b}_1, \mathbf{a}_2 \otimes \mathbf{b}_2, \ldots, \mathbf{a}_{n_3} \otimes \mathbf{b}_{n_3}]$. We use $\mathbf{A} \circ \mathbf{B}$ to denote the *Hadamard product* (entry-wise product) of matrices $\mathbf{A}$ and $\mathbf{B}$ of the same size, i.e., $[\mathbf{A} \circ \mathbf{B}]_{ij} = \mathbf{A}_{ij}\mathbf{B}_{ij}$. We also denote their corresponding powers by $\mathbf{a}^{\otimes l}$, $\mathbf{A}^{\odot l}$ and $\mathbf{A}^{\circ l}$.

Recall $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n) \in \mathbb{R}^{d \times n}$. Let $\mathbf{K} = \mathbf{X}^\top\mathbf{X} \in \mathbb{R}^{n \times n}$. Then it is easy to see that $[\mathbf{K}^{\circ l}]_{ij} = \mathbf{K}_{ij}^l = \langle \mathbf{x}_i, \mathbf{x}_j \rangle^l$ and $\mathbf{K}^{\circ l} = (\mathbf{X}^{\odot l})^\top \mathbf{X}^{\odot l} \succeq \mathbf{0}$ for all $l \in \mathbb{N}$. Recall from (3) that $\mathbf{H}_{ij}^\infty = \frac{\mathbf{K}_{ij}}{4} + \frac{\mathbf{K}_{ij}\arcsin(\mathbf{K}_{ij})}{2\pi}$. Since $\arcsin(x) = \sum_{l=0}^\infty \frac{(2l-1)!!}{(2l)!!} \cdot \frac{x^{2l+1}}{2l+1}$ $(|x| \leq 1)$[7], we have

$$\mathbf{H}_{ij}^\infty = \frac{\mathbf{K}_{ij}}{4} + \frac{1}{2\pi}\sum_{l=1}^\infty \frac{(2l-3)!!}{(2l-2)!!} \cdot \frac{\mathbf{K}_{ij}^{2l}}{2l-1},$$

which means

$$\mathbf{H}^\infty = \frac{\mathbf{K}}{4} + \frac{1}{2\pi}\sum_{l=1}^\infty \frac{(2l-3)!!}{(2l-2)!!} \cdot \frac{\mathbf{K}^{\circ 2l}}{2l-1}.$$

Since $\mathbf{K}^{\circ l} \succeq \mathbf{0}$ $(\forall l \in \mathbb{N})$, we have $\mathbf{H}^\infty \succeq \frac{\mathbf{K}}{4}$ and

$$\mathbf{H}^\infty \succeq \frac{1}{2\pi}\frac{(2l-3)!!}{(2l-2)!!} \cdot \frac{\mathbf{K}^{\circ 2l}}{2l-1} \succeq \frac{\mathbf{K}^{\circ 2l}}{2\pi(2l-1)^2}, \quad \forall l \in \mathbb{N}_+.$$

Now we proceed to prove the theorem.

First we consider the case $p = 1$. In this case we have $\mathbf{y} = \alpha\mathbf{X}^\top\boldsymbol{\beta}_1$. Since $\mathbf{H}^\infty \succeq \frac{\mathbf{K}}{4}$, from Lemma E.1 we have

$$\mathbf{P}_\mathbf{K}(\mathbf{H}^\infty)^{-1}\mathbf{P}_\mathbf{K} \preceq 4\mathbf{K}^\dagger,$$

where $\mathbf{P}_\mathbf{K} = \mathbf{K}^{1/2}\mathbf{K}^\dagger\mathbf{K}^{1/2}$ is the projection matrix for the subspace spanned by $\mathbf{K}$. Since $\mathbf{K} = \mathbf{X}^\top\mathbf{X}$, we have $\mathbf{P}_\mathbf{K}\mathbf{X}^\top = \mathbf{X}^\top$. Therefore, we have

$$\begin{aligned}
&\mathbf{y}^\top(\mathbf{H}^\infty)^{-1}\mathbf{y} \\
=&\alpha^2\boldsymbol{\beta}^\top\mathbf{X}(\mathbf{H}^\infty)^{-1}\mathbf{X}^\top\boldsymbol{\beta} \\
=&\alpha^2\boldsymbol{\beta}^\top\mathbf{X}\mathbf{P}_\mathbf{K}(\mathbf{H}^\infty)^{-1}\mathbf{P}_\mathbf{K}\mathbf{X}^\top\boldsymbol{\beta}
\end{aligned}$$

[7] $p!! = p(p-2)(p-4)\cdots$ and $0!! = (-1)!! = 1$.

$$
\begin{aligned}
&\leq 4\alpha^2 \boldsymbol{\beta}^\top \mathbf{X}\mathbf{K}^\dagger \mathbf{X}^\top \boldsymbol{\beta} \\
&= 4\alpha^2 \boldsymbol{\beta}^\top \mathbf{P}_{\mathbf{X}\mathbf{X}^\top} \boldsymbol{\beta} \\
&\leq 4\alpha^2 \left\|\boldsymbol{\beta}\right\|_2^2 .
\end{aligned}
$$

This finishes the proof for $p = 1$.

Similarly, for $p = 2l$ ($l \in \mathbb{N}_+$), we have $\mathbf{y} = \alpha \left(\mathbf{X}^{\odot 2l}\right)^\top \boldsymbol{\beta}^{\otimes 2l}$. From $\mathbf{H}^\infty \succeq \frac{\mathbf{K}^{\circ 2l}}{2\pi(2l-1)^2} = \frac{(\mathbf{X}^{\odot 2l})^\top \mathbf{X}^{\odot 2l}}{2\pi(2l-1)^2}$ and Lemma E.1 we have

$$
\begin{aligned}
&\mathbf{y}^\top (\mathbf{H}^\infty)^{-1} \mathbf{y} \\
=& \alpha^2 (\boldsymbol{\beta}^{\otimes 2l})^\top \mathbf{X}^{\odot 2l} (\mathbf{H}^\infty)^{-1} (\mathbf{X}^{\odot 2l})^\top \boldsymbol{\beta}^{\otimes 2l} \\
\leq& 2\pi(2l-1)^2 \alpha^2 (\boldsymbol{\beta}^{\otimes 2l})^\top \mathbf{X}^{\odot 2l} (\mathbf{K}^{\circ 2l})^\dagger (\mathbf{X}^{\odot 2l})^\top \boldsymbol{\beta}^{\otimes 2l} \\
=& 2\pi(2l-1)^2 \alpha^2 (\boldsymbol{\beta}^{\otimes 2l})^\top \mathbf{P}_{\mathbf{X}^{\odot 2l}(\mathbf{X}^{\odot 2l})^\top} \boldsymbol{\beta}^{\otimes 2l} \\
\leq& 2\pi(2l-1)^2 \alpha^2 \left\|\boldsymbol{\beta}^{\otimes 2l}\right\|_2^2 \\
=& 2\pi(2l-1)^2 \alpha^2 \left\|\boldsymbol{\beta}\right\|_2^{4l} \\
\leq& 2\pi p^2 \alpha^2 \left\|\boldsymbol{\beta}\right\|_2^{2p} .
\end{aligned}
$$

This finishes the proof for $p = 2l$. □