Understanding Why Generalized Reweighting Does Not Improve Over ERM

Runtian Zhai 1  Chen Dan 1  J. Zico Kolter 1  Pradeep Ravikumar 1

Abstract
Empirical risk minimization (ERM) is known in practice to be non-robust to distributional shift where the training and the test distributions are different. A suite of approaches, such as importance weighting, and variants of distributionally robust optimization (DRO), have been proposed to solve this problem. But a line of recent work has empirically shown that these approaches do not significantly improve over ERM in real applications with distribution shift. The goal of this work is to obtain a comprehensive theoretical understanding of this intriguing phenomenon. We first posit the class of Generalized Reweighting (GRW) algorithms, as a broad category of approaches that iteratively update model parameters based on iterative reweighting of the training samples. We show that when overparameterized models are trained under GRW, the resulting models are close to that obtained by ERM. We also show that adding small regularization which does not greatly affect the empirical training accuracy does not help. Together, our results show that a broad category of what we term GRW approaches are not able to achieve distributionally robust generalization. Our work thus has the following sobering takeaway: to make progress towards distributionally robust generalization, we either have to develop non-GRW approaches, or perhaps devise novel classification/regression loss functions that are adapted to the class of GRW approaches.

1. Introduction
It has now been well established that empirical risk minimization (ERM) can empirically achieve high test performance on a variety of tasks, particularly with modern overparameterized models where the number of parameters is much larger than the number of training samples. This strong performance of ERM however has been shown to degrade under distributional shift, where the training and test distributions are different (Hovy & Søgaard, 2015; Blodgett et al., 2016; Tatman, 2017).

There are two broad categories of distribution shift studied in recent years. The first is domain generalization, where the training distribution is a mixture of environments, while the test distribution contains new environments that do not appear in the training distribution. The hope in such cases is to learn “invariant features” that do not change across environments, in contrast to spurious features, such as the background in image classification instead of the object, and negation words such as “not” and “never” in language sentiment analysis instead of the sentence meaning itself. However, it has been empirically shown that overparameterized models trained via ERM tend to learn spurious features. The second is subpopulation shift, where the training distribution consists of a number of groups, and the test distribution is the group-conditional distribution of any group (or more generally, an arbitrary mixture of the training groups). Such subpopulation shift occurs in the context of fair machine learning, where the dataset is divided into demographic groups, and it is of interest to perform well on all such groups; as well as in learning with imbalanced classes, where each class is a group, and the model needs to perform well on all classes. While overparameterized models trained via ERM can achieve high average performance over the entire data domain, they have been shown to have low performance on underrepresented data subpopulations.

People have proposed various approaches to learn models that are robust to such distributional shift. The most classical approach is importance weighting (Shimodaira, 2000), which reweights training samples so that each group has the same overall weight in the training objective. The approach most widely used today is Distributional Robust Optimization (DRO) (Duchi & Namkoong, 2018; Hashimoto et al., 2018), in which we assume that the test distribution belongs to a certain set of distributions that are close to the training distribution, and train the model on the worst distribution in that set. Many variants of DRO have been proposed and are used in practice (Hu et al., 2018; Sagawa et al., 2020a; Xu et al., 2020; Zhai et al., 2021a,b).

While these approaches have been developed for the express...
purpose of improving ERM for distribution shift, a line of recent work has empirically shown the negative result that when used to train overparameterized models, these methods do not improve over ERM. For importance weighting, (Byrd & Lipton, 2019) observed that its effect under stochastic gradient descent (SGD) diminishes over training epochs, and finally does not improve over ERM. For variants of DRO, (Sagawa et al., 2020a) found that these overfit very easily, i.e. the performance on the test distribution will drop to the same low level as ERM after sufficiently many epochs if no regularization is applied. (Gulrajani & Lopez-Paz, 2021; Koh et al., 2021) compared these methods with ERM on a number of real-world applications, and found that in most cases none of these methods improves over ERM.

This line of empirical results has also been bolstered by some recent theoretical results. (Sagawa et al., 2020b) constructed a synthetic dataset where a linear model trained with importance weighting is provably not robust to subpopulation shift. (Xu et al., 2021) further proved that under gradient descent (GD) with a sufficiently small learning rate, a linear classifier trained with either importance weighting or ERM converges to the same max-margin classifier, and thus upon convergence, are no different. These previous theoretical results are limited to linear models and the specific approaches where sample weights are fixed during training. They are not applicable to more complex models, and more general approaches where the sample weights could iteratively change, including most DRO variants.

Towards placing the line of empirical results on a stronger theoretical footing, we first define the class of generalization reweighting (GRW), which assigns each sample a weight that could vary with training iterations, and iteratively minimizing the weighted average loss (instead of the average loss as in ERM). By allowing the weights to vary with iterations, we cover not just ERM and static importance weighting, but also DRO approaches outlined earlier; though of course, the GRW class is much broader than just these instances.

In this work, we show the comprehensive result that in both regression and classification, and for both overparameterized linear and wide neural networks, the models learnt via any GRW approach and ERM are similar, in the sense that their implicit biases are (almost) equivalent. We note that extending the analysis from linear models to wide neural networks is non-trivial since it requires the approximation result that wide neural networks can be approximated by their linearized counterparts to hold uniformly throughout the iterative process of the general class of GRW algorithms. Our results extend the analysis in (Lee et al., 2019), but as we show, the proof in the original paper had some flaws, and due to which we had to fix the proof by changing the network initialization (Eqn. (11), see Appendix E).

Overall, our results provide the important takeaway that distributionally robust generalization cannot be directly achieved by the broad class of GRW algorithms (which includes popular approaches such as importance weighting and most DRO variants). Progress towards this important goal thus requires either going beyond GRW algorithms, or devising novel loss functions that are adapted to the class of GRW approaches (see Appendix B).

2. Preliminaries

Let the input space be $\mathcal{X} \subseteq \mathbb{R}^d$ and the output space be $\mathcal{Y} \subseteq \mathbb{R}$.\(^1\) For our theoretical analysis, we assume that the input space $\mathcal{X}$ is a subset of the unit $L_2$ ball of $\mathbb{R}^d$, such that any $x \in \mathcal{X}$ satisfies $\|x\|_2 \leq 1$. We are given a training set $\{z_i = (x_i, y_i)\}_{i=1}^n$ i.i.d. sampled from an underlying training distribution $P$ over $\mathcal{X} \times \mathcal{Y}$. Denote $X = (x_1, \cdots, x_n) \in \mathbb{R}^{d \times n}$, and $Y = (y_1, \cdots, y_n) \in \mathbb{R}^n$; for any function $g : \mathcal{X} \mapsto \mathbb{R}^m$, we overload the notation and use $g(X) = (g(x_1), \cdots, g(x_n)) \in \mathbb{R}^{m \times n}$ (except when $m = 1$, $g(X)$ is defined as a column vector). Let the loss function be $\ell : \mathcal{Y} \times \mathcal{Y} \mapsto [0, 1]$. ERM trains a model by minimizing its expected risk:

$$
\mathcal{R}(f; P) = \mathbb{E}_{x \sim P}[\ell(f(x), y)]
$$

via minimizing the empirical risk:

$$
\hat{\mathcal{R}}(f) = \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i)
$$

In distributional shift, the model is evaluated not on the training distribution $P$, but a different test distribution $P_{\text{test}}$, so that we care about the expected risk $\mathcal{R}(f; P_{\text{test}})$. A large family of methods designed for such distributional shift is distributionally robust optimization (DRO), which minimizes the expected risk over the worst-case distribution $Q \ll P$ in a ball w.r.t. divergence $D$ around the training distribution $P$. Specifically, DRO minimizes the expected DRO risk defined as:

$$
\mathcal{R}_{D, \rho}(f; P) = \sup_{Q \ll P} \{\mathbb{E}_Q[\ell(f(x), y)] : D(Q \parallel P) \leq \rho\}
$$

(3)

for some $\rho > 0$. Instances of such DRO risk include CVaR, \(\chi^2\)-DRO (Hashimoto et al., 2018), and DORO (Zhai et al., 2021a), among others.

A common category of distribution shift is known as subpopulation shift. Let the data domain contain $K$ groups $D_1, \cdots, D_K$. The training distribution $P$ is the distribution over all groups, and the test distribution $P_{\text{test}}$ is the distribution over one of the groups. Let $P_k(z) = P(z \mid z \in D_k)$

\(^1\)For simplicity we prove our results for $\mathcal{Y} \subseteq \mathbb{R}$, but they can be easily extended to the multi-class scenario (see Appendix B.3).

\(^2\)For distributions $P$ and $Q$, $Q$ is absolute continuous to $P$, or $Q \ll P$, means that for any event $A$, $P(A) = 0$ implies $Q(A) = 0$. This also means that $Q$ has the same support as $P$. 

For distributions $P$ and $Q$, we say $P$ is absolute continuous to $Q$, or $P \ll Q$, if for all measurable functions $f : \mathcal{X} \mapsto \mathbb{R}$, $f$ is measurable  with respect to $P$ if and only if $f$ is measurable with respect to $Q$.
be the conditional distribution over group \( k \), then \( P_{\text{test}} \) can be any one of \( P_1, \ldots, P_k \). The goal is to train a model \( f \) that performs well over every group. There are two common ways to achieve this goal: one is minimizing the balanced empirical risk which is an unweighted average of the empirical risk over each group, and the other is minimizing the worst-group risk defined as

\[
\mathcal{R}_{\text{max}}(f; P) = \max_{k=1,\ldots,K} \mathcal{R}(f; P_k) = \max_{k=1,\ldots,K} \mathbb{E}_{z \sim P}[\ell(f(x), y) | z \in \mathcal{D}_k]
\]  

(4)

3. Generalized Reweighting (GRW)

As mentioned before, a number of methods have been proposed towards learning models that are robust to distributional shift. In contrast to analyzing each of these individually, we instead consider a large class of what we call Generalized Reweighting (GRW) algorithms that includes the ones we have discussed earlier, but potentially many others more. Loosely, GRW algorithms iteratively assign each sample a weight during training (that could vary with the iteration) and iteratively minimize the weighted average risk. Specifically, at iteration \( t \) GRW assigns a weight \( q^{(t)} \) to sample \( z_i \), and minimizes the weighted empirical risk:

\[
\hat{\mathcal{R}}_{q^{(t)}}(f) = \sum_{i=1}^{n} q^{(t)}_{i} \ell(f(x_i), y_i)
\]  

(5)

where \( q^{(t)} = (q^{(t)}_1, \ldots, q^{(t)}_n) \) and \( q^{(t)}_1 + \cdots + q^{(t)}_n = 1 \).

Static GRW assigns to each \( z_i = (x_i, y_i) \) a fixed weight \( q_i \) that does not change during training, i.e. \( q^{(t)}_i = q_i \). A classical method is importance weighting (Shimodaira, 2000), where if \( z_i \in \mathcal{D}_k \) and the size of \( \mathcal{D}_k \) is \( n_k \), then \( q_i = (\mathcal{D} n_k)^{-1} \). Under importance weighting, (5) becomes the balanced empirical risk in which each group has the same weight. Note that ERM is also a special case of static GRW: by assigning \( q_i = \cdots = q_n = 1/n \).

On the other hand, in dynamic GRW, \( q^{(t)} \) changes with \( t \). For instance, any approach that iteratively upweights samples where the model has high losses in order to help the model learn “hard” samples is an instance of GRW. Algorithms that implement DRO fall under this category as well. When estimating the population DRO risk \( \mathcal{R}_{\mathcal{D},\rho}(f; P) \) in Eqn. (3), if \( P \) is set to the distribution over the training samples, then \( Q \ll P \) implies that \( Q \) is also a distribution over the training samples. Thus, DRO methods belong to the broad class of GRW algorithms. There are two major ways to implement DRO. One uses Danskin’s theorem and chooses \( Q \) as the maximizer of \( \mathbb{E}_{Q}[\ell(f(x), y)] \) in each epoch. The other one is to formulate DRO as a bilevel optimization problem, where the lower layer updates the model to minimize the expected risk over \( Q \), and the upper layer updates \( Q \) to maximize it. Both can be seen as instances of GRW. As one popular instance of the latter, Group DRO was proposed by (Sagawa et al., 2020a) to minimize (4). Denote the empirical risk over group \( k \) by \( \hat{\mathcal{R}}_{k}(f) \), and the model at time \( t \) by \( f^{(t)} \). Group DRO iteratively sets \( q^{(t)}_i = q^{(t)}_k / n_k \) for all \( z_i \in \mathcal{D}_k \) where \( g^{(t)}_k \) is the group weight that is updated as

\[
g^{(t)}_k \propto g^{(t-1)}_k \exp \left( \nu \hat{\mathcal{R}}_{k}(f^{(t-1)}) \right) \quad (\forall k = 1, \ldots, K)
\]  

(6)

for some \( \nu > 0 \), and then normalized so that \( q^{(t)}_1 + \cdots + q^{(t)}_n = 1 \). (Sagawa et al., 2020a) then showed (in their Proposition 2) that for convex settings, the Group DRO risk of iterates converges to the global minimum with the rate \( O(t^{-1/2}) \) if \( \nu \) is sufficiently small.

4. Theoretical Results for Regression

In this section, we will study GRW for regression tasks that use the squared loss

\[
\ell(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2.
\]  

(7)

We will prove that for both linear models and sufficiently wide fully-connected neural networks, the implicit bias of GRW is equivalent to ERM, so that starting from the same initial point, GRW and ERM will converge to the same point when trained for an infinitely long time, which explains why GRW does not improve over ERM without regularization and early stopping. We will further show that while regularization can affect this implicit bias, it must be large enough to significantly lower the training performance, or the final model will still be close to the unregularized ERM model.

4.1. Linear Models

We first demonstrate our result on simple linear models to provide our readers with a key intuition; later, we will apply this same intuition to neural networks. This key intuition draws from results of (Gunasekar et al., 2018). Let the linear model be denoted by \( f(x) = \langle \theta, x \rangle \), where \( \theta \in \mathbb{R}^d \). We consider the overparameterized setting where \( d > n \). The weight update rule of GRW under GD is the following:

\[
\theta^{(t+1)} = \theta^{(t)} - \eta \sum_{i=1}^{n} q^{(t)}_i \nabla \ell(f^{(t)}(x_i), y_i)
\]  

(8)

where \( \eta > 0 \) is the learning rate. For a linear model with the squared loss, the update rule is

\[
\theta^{(t+1)} = \theta^{(t)} - \eta \sum_{i=1}^{n} q^{(t)}_i (x_i f^{(t)}(x_i) - y_i)
\]  

(9)

For this training scheme, we can prove for any GRW, if the training error converges to zero, then the model con-
verges to an interpolator \( \theta^* \) (such that for all \( i \), \( \langle \theta^*, x_i \rangle = y_i \)) independent of \( q_i \) (see the proofs in Appendix D):

**Theorem 4.1.** If \( x_1, \ldots, x_n \) are linearly independent, then under the squared loss, for any GRW such that the empirical training risk \( \mathcal{R}(f^{(l)}) \to 0 \) as \( t \to \infty \), it holds that \( \theta^{(l)} \) converges to an interpolator \( \theta^* \) that only depends on \( \theta^{(0)} \) but does not depend on \( q_i^{(l)} \).

The proof is based on the following key intuition regarding the update rule (9): \( \theta^{(l+1)} - \theta^{(l)} \) is a linear combination of \( x_1, \ldots, x_n \) for all \( t \), so \( \theta^{(t)} - \theta^{(0)} \) always lies in the linear subspace \( \text{span}\{x_1, \ldots, x_n\} \), which is an \( n \)-dimensional linear subspace if \( x_1, \ldots, x_n \) are linearly independent. By Cramer’s rule, there is exactly one \( \theta \) in this subspace such that we get interpolation of all the data \( \langle \theta + \theta^{(0)}, x_i \rangle = y_i \) for all \( i \in \{1, \ldots, n\} \). In other words, the parameter \( \theta^* = \theta + \theta^{(0)} \) in this subspace that interpolates all the data is unique. Thus the proof would follow if we were to show that \( \theta^{(t)} - \theta^{(0)} \), which lies in the subspace, also converges to interpolating the data. Here the linear independence of \( x_1, \ldots, x_n \) is necessary, because otherwise in the extreme case where \( x_1 = x_2 \) but \( y_1 \neq y_2 \), the model cannot fit both \( (x_1, y_1) \) and \( (x_2, y_2) \).

We have essentially proved the following sobering result: the implicit bias of any GRW that achieves zero training error is equivalent to ERM, so GRW does not improve over ERM. While the various distributional shift methods discussed in the introduction have been shown to have such convergence with overparameterized models and linearly independent inputs (Sagawa et al., 2020a), we provide the following theorem that shows this for the broad class of GRW methods. Specifically, we show that for any GRW satisfying the following assumption, its training error converges to 0 with a sufficiently small learning rate:

**Assumption 1.** There exist constants \( q_1, \ldots, q_n \) such that for all \( i \), \( q_i^{(l)} \to q_i \) as \( t \to \infty \). And \( \min_i q_i = q^* > 0 \).

**Theorem 4.2.** If \( x_1, \ldots, x_n \) are linearly independent, then there exists \( \eta_0 > 0 \) such that for any GRW satisfying Assumption 1 with the squared loss, and any \( \eta < \eta_0 \), the empirical training risk \( \mathcal{R}(f^{(l)}) \to 0 \) as \( t \to \infty \).

As just one example, all static GRW methods, which includes importance weighting as well as ERM, vacuously satisfy Assumption 1.

However, as (Gunasekar et al., 2018) have also pointed out, the key intuition above on data interpolators only works for “losses with a unique finite root” such as the squared loss. For example, when trained with the logistic loss, the model cannot converge to a finite interpolator, so the intuition is not applicable. In Section 5 we will show how to extend our results to such losses.

**4.2. Wide Neural Networks**

Now we study sufficiently wide fully-connected neural networks. We extend the analysis in (Lee et al., 2019) in the neural tangent kernel (NTK) regime (Jacot et al., 2018). The neural network we study has the following formulation:

\[
\begin{align*}
    h_{t+1}^{l} & = \frac{W_{t}^{l}}{\sqrt{d_{l}}} x^{l} + \beta b^{l} \quad (l = 0, \ldots, L) \\
    x_{t+1}^{l} & = \sigma(h_{t+1}^{l}) \quad (l = 0, \ldots, L)
\end{align*}
\]

where \( \sigma \) is a non-linear activation function, \( W_{t}^{l} \in \mathbb{R}^{d_{l+1} \times d_{l}} \) and \( W_{t}^{L} \in \mathbb{R}^{1 \times d_{1}} \). Here \( d_{0} = d \). The parameter vector \( \theta \) consists of \( W^{0}, \ldots, W^{L} \) and \( b^{0}, \ldots, b^{L} \) (\( \theta \) is the concatenation of all flattened weights and biases). The final output of the neural network is \( f(x) = h_{L+1}^{1} \). And let the neural network be initialized as

\[
\begin{align*}
    W_{t}^{l,i} & \sim \mathcal{N}(0, 1) \quad (l = 0, \ldots, L - 1) \\
    b_{t}^{l,i} & \sim \mathcal{N}(0, 1) \\
    W_{L}^{l,i} & = 0 \\
    b_{L}^{l,i} & \sim \mathcal{N}(0, 1)
\end{align*}
\]

We also need the following assumption on the wide NN:

**Assumption 2.** \( \sigma \) is differentiable everywhere, and both \( \sigma \) and \( \sigma ' \) Lipschitz.

**Difference from (Jacot et al., 2018).** Our initialization (11) differs from the original one in (Jacot et al., 2018) in the last (output) layer. For the output layer, we use the zero initialization \( W_{L}^{L,i} = 0 \) instead of the Gaussian initialization \( W_{L}^{L,i} \sim \mathcal{N}(0, 1) \). This modification enables us to accurately approximate the neural network with its linearized counterpart (13), as we notice that the proofs in (Lee et al., 2019) (particularly the proofs of their Theorem 2.1 and their Lemma 1 in Appendix G) are flawed. In Appendix E we explain what goes wrong in their proofs and how we manage to fix the proofs with our modification.

Denote the neural network at time \( t \) by \( f^{(l)}(x) = f(x; \theta^{(l)}) \) which is parameterized by \( \theta^{(l)} \in \mathbb{R}^{p} \) where \( p \) is the number of parameters. We use the shorthand \( \nabla_{\theta} f^{(l)}(x) := \nabla_{\theta} f(x; \theta) \big|_{\theta = \theta_{0}} \). The neural tangent kernel (NTK) of this model is \( \Theta^{(0)}(x, x') = (\nabla_{\theta} f^{(0)}(x)^{T} \nabla_{\theta} f^{(0)}(x')) \), and the Gram matrix is \( \Theta^{(0)}(X, X) = \Theta^{(0)}(\mathbb{R}, \mathbb{R}) \). For the wide neural network with our new initialization, we still have the following NTK theorem:

**Lemma 4.3.** If \( \sigma \) is Lipschitz and \( d_{i} \to \infty \) for \( l = 1, \ldots, L \) sequentially, then \( \Theta^{(0)}(x, x') \) converges in probability to a non-degenerated\(^4\) deterministic limiting kernel \( \Theta(x, x') \).

\(^{3}\) \( f \) is Lipschitz if there exists a constant \( L > 0 \) such that for any \( x_1, x_2, |f(x_1) - f(x_2)| \leq L \|x_1 - x_2\|_2 \).

\(^{4}\) Non-degenerated means that \( \Theta(x, x') \) depends on \( x \) and \( x' \) and is not a constant.
The kernel Gram matrix $\Theta = \Theta(X, X) \in \mathbb{R}^{n \times n}$ is a positive semi-definite symmetric matrix. Denote its largest and smallest eigenvalues by $\lambda_{\text{max}}$ and $\lambda_{\text{min}}$. Note that $\Theta$ is non-degenerated, so we can assume that $\lambda_{\text{min}} > 0$ (which is almost surely true in the overparameterized setting where $d_L \gg n$). The main theorem of this section is the following:

**Theorem 4.4.** For a wide fully-connected neural network $f(t)$ that satisfies Assumption 2 and is trained by any GRW satisfying Assumption 1 with the squared loss, if $d_1 = d_2 = \cdots = d_L = d$, $\lambda_{\text{max}} > 0$, and $\nabla f(0)(x_1), \cdots, \nabla f(0)(x_n)$ are linearly independent, then there exists a constant $\eta_1 > 0$ such that: if $\eta \leq \eta_1$, then for any $\delta > 0$, there exist a constant $D > 0$ such that as long as $d \geq D$, with probability at least $(1 - \delta)$ over random initialization we have: for any test point $x \in \mathbb{R}^d$ such that $\|x\|_2 \leq 1$, as $d \rightarrow \infty$,

$$\limsup_{t \rightarrow \infty} \left| f(t)(x) - f(t)_{\text{ERM}}(x) \right| = O(d^{-1/4}) \rightarrow 0$$

where $f(t)$ is trained by GRW and $f(t)_{\text{ERM}}$ is trained by ERM, and both models start from the same initial point.

Note that for simplicity, in the theorem we only consider the case where $d_1 = \cdots = d_L = d \rightarrow \infty$, but in fact the result can be very easily extended to the case where $d_1/d_2/\cdots/\alpha_l$ for $l = 2, \cdots, L$ for some constants $\alpha_2, \cdots, \alpha_L$, and $d_1 \rightarrow \infty$. Here we provide a proof sketch for this theorem. The key is to consider the linearized neural network of $f(t)(x)$:

$$f_{\text{lin}}(t)(x) = f(0)(x) + (\theta(t) - \theta(0), \nabla f(0)(x))$$

which is a linear model with features $\nabla f(0)(x)$. Thus if $\nabla f(0)(x_1), \cdots, \nabla f(0)(x_n)$ are linearly independent, then the linearized NN converges to the unique interpolator. Then we show that the wide neural network can be approximated by its linearized counterpart uniformly throughout training, which is considerably more subtle in our case due to the GRW dynamics. Here we prove that the gap between the two models is bounded by $O(d^{-1/4})$, but in fact we can prove that it is bounded by $O(d^{-1/2-\epsilon})$ for any $\epsilon > 0$.

**Lemma 4.5** (Approximation Theorem). For a wide fully-connected neural network $f(t)$ satisfying Assumption 2 and is trained by any GRW satisfying Assumption 1 with the squared loss, let $f_{\text{lin}}(t)$ be its linearized neural network trained by the same GRW (i.e. $q(t)$ are the same for both networks for any $i$ and $t$). Under the conditions of Theorem 4.4, with a sufficiently small learning rate, for any $\delta > 0$, there exist constants $D > 0$ and $C > 0$ such that as long as $d \geq D$, with probability at least $(1 - \delta)$ over random initialization we have: for any test point $x \in \mathbb{R}^d$ such that $\|x\|_2 \leq 1$,

$$\sup_{t \geq 0} \left| f_{\text{lin}}(t)(x) - f(t)(x) \right| \leq C d^{-1/4}$$

(14)

To make results easier to understand, in later results this condition will be written as “with a sufficiently small learning rate”.

Theorem 4.4 shows that at any test point $x$ within the unit ball, the gap between the outputs of wide NNs trained by GRW and ERM from the same initial point is arbitrarily close to 0. So we have shown that for regression, with both linear and wide NNs, GRW does not improve over ERM.

**4.3. Wide Neural Networks, with $L_2$ Regularization**

Previous work such as (Sagawa et al., 2020a) proposed to improve DRO algorithms by adding $L_2$ penalty to the objective function. In this section, we thus study adding $L_2$ regularization to the broad class of GRW algorithms:

$$\tilde{\mathcal{R}}_q^{\mu}(f) = \sum_{i=1}^{n} q_i(t) \ell(f(x_i), y_i) + \frac{\mu}{2} \|\theta - \theta(0)\|_2^2$$

(15)

From the outset, it is easy to see that under $L_2$ regularization, GRW methods have different implicit biases than ERM. For example, when $f$ is a linear model, $\ell$ is convex and smooth, then $\tilde{\mathcal{R}}_q^{\mu}(f)$ with static GRW is a convex smooth objective function, so under GD with a sufficiently small learning rate, the model will converge to the global minimizer (see Appendix D.1). Moreover, the global optimum $\theta^*$ satisfies $\nabla \theta \tilde{\mathcal{R}}_q^{\mu}(f(x; \theta^*)) = 0$, solving which yields

$$\theta^* = \theta(0) + (JQJ^T + \mu I)^{-1}JQ(Y - f(0)(X))$$

(16)

which depends on $Q$, so adding $L_2$ regularization at least seems to yield results that are different from ERM (whether it improves over ERM might depend on the weights $Q$).

However, the following result shows that this regularization must be large enough to significantly lower the training performance, or the resulting model would still be very close to the unregularized ERM model. We still denote the largest and smallest eigenvalues of the kernel Gram matrix $\Theta$ by $\lambda_{\text{max}}$ and $\lambda_{\text{min}}$. We use the subscript “reg” to refer to a regularized model (trained by minimizing (15)).

**Theorem 4.6.** Suppose there exists $M_0 > 0$ such that $\|\nabla f(0)(x)\|_2 \leq M_0$ for all $\|x\|_2 \leq 1$. If $\lambda_{\text{max}} > 0$ and $\mu > 0$, then for a wide NN satisfying Assumption 2, and any GRW minimizing the squared loss with a sufficiently small learning rate $\eta$, if $d_1 = d_2 = \cdots = d_L = d$, $\nabla f(0)(x_1), \cdots, \nabla f(0)(x_n)$ are linearly independent, and the empirical training risk of $f_{\text{reg}}(t)$ satisfies

$$\limsup_{t \rightarrow \infty} \tilde{\mathcal{R}}_q^{\mu}(f_{\text{reg}}(t)) < \epsilon$$

(17)

for some $\epsilon > 0$, then with a sufficiently small learning rate, as $d \rightarrow \infty$, with probability close to 1 over random initialization, for any $x$ such that $\|x\|_2 \leq 1$ we have

$$\limsup_{t \rightarrow \infty} \left| f_{\text{reg}}(t)(x) - f_{\text{ERM}}(t)(x) \right| = O(d^{-1/4} + \sqrt{\epsilon}) \rightarrow O(\sqrt{\epsilon})$$

(18)

where $f_{\text{reg}}(t)$ is trained by regularized GRW and $f_{\text{ERM}}(t)$ by unregularized ERM, and both start from the same point.
The proof again starts from analyzing linearized neural networks, and showing that regularization does not help there (Appendix D.4.2). Then, to extend the results to wide neural networks, we need to prove a new approximation theorem for $L_2$ regularized GRW connecting wide NNs to their linearized counterparts uniformly through the GRW training process (Appendix D.4.1). Note that with regularization, we no longer need Assumption 1 to prove the new approximation theorem. This is because in the proof of Lemma 4.5, Assumption 1 is used as a sufficient condition for the convergence of the wide neural network GRW iterates, but with regularization the GRW iterates naturally converge.

Theorem 4.6 shows that if the training error can go below $\epsilon$, then the gap between the two models on any test point $x$ within the unit ball will be at most $O(\sqrt{\epsilon})$. Thus, if $\epsilon$ is very small, regularized GRW yields a very similar model to unregularized ERM, and hence cannot improve over ERM with respect to distributional shift.

5. Theoretical Results for Classification

Now we consider classification tasks where $Y = \{+1, -1\}$. The fundamental difference is that classification losses do not have finite minimizers. A classification loss converging to zero means that the model weight “explodes” to infinity, unlike in regression where the model converges to a finite interpolator. We focus on the canonical logistic loss:

$$\ell(\hat{y}, y) = \log(1 + \exp(-\hat{y}y)) \quad (19)$$

5.1. Linear Models

We first consider training the linear model $f(x) = \langle \theta, x \rangle$ with GRW under gradient descent with the logistic loss. As noted earlier, in this setting of linear models for classification, (Byrd & Lipton, 2019) had made the empirical observation that importance weighting does not improve over ERM. Then, (Xu et al., 2021) proved that for importance weighting algorithms, as $t \to \infty$, $\|\theta(t)\|_2 \to \infty$ and $\theta(t) / \|\theta(t)\|_2$ converges to a unit vector that does not depend on the sample weights, so it does not improve over ERM. To extend this theoretical result to the broad class of GRW algorithms, we will prove two results. First, in Theorem 5.1 we will show that under the logistic loss, any GRW algorithm satisfying the following weaker assumption:

**Assumption 3.** For all $i$, $\lim \inf_{t \to \infty} q_i^{(t)} > 0$,

if the training error converges to 0, and the direction of the model weight converges to a fixed unit vector, then this unit vector must be the max-margin classifier defined as

$$\hat{\theta}_{MM} = \arg \max_{\theta : \|\theta\|_2 = 1} \left\{ \min_{i=1, \ldots, n} y_i \cdot \langle \theta, x_i \rangle \right\} \quad (20)$$

Second, Theorem 5.2 shows that for any GRW satisfying Assumption 1, the training error converges to 0 and the direction of the model weight converges. Hence any GRW satisfying Assumption 1 does not improve over ERM.

**Theorem 5.1.** If $x_1, \ldots, x_n$ are linearly independent, then for the logistic loss, with a sufficiently small learning rate $\eta$ we have: for any GRW satisfying Assumption 3, if as $t \to \infty$ the empirical training risk $R_t(f^{(t)})$ converges to 0 and $\theta(t) / \|\theta(t)\|_2 \to u$ for some unit vector $u$, then $u = \hat{\theta}_{MM}$.

This result is an extension of (Soudry et al., 2018). Note that $\hat{\theta}_{MM}$ does not depend on $q_i^{(t)}$, so this result shows that the reweighting has no effect on the implicit bias. We thus have the sobering result that any GRW method that only satisfies the weak Assumption 3, as long as the training error converges to 0 and the model weight direction converges, GRW does not improve over ERM. We next show that any GRW satisfying Assumption 1 does have its model weight direction converge, and its training error converge to 0.

**Theorem 5.2.** For any loss $\ell$ that is convex, differentiable, $L$-smooth in $\hat{y}$ and strictly monotonically decreasing to zero as $\hat{y} \to +\infty$, and GRW satisfying Assumption 1, denote

$$F(\theta) = \sum_{i=1}^n q_i \ell(\langle \theta, x_i \rangle, y_i) \quad (21)$$

If $x_1, \ldots, x_n$ are linearly independent, then with a sufficiently small learning rate $\eta$, we have:

(i) $F(\theta(t)) \to 0$ as $t \to \infty$.

(ii) $\|\theta(t)\|_2 \to \infty$ as $t \to \infty$.

(iii) Define $\theta_R = \arg \min_{\theta : \|\theta\|_2 \leq R} \{ F(\theta) : \|\theta\|_2 \leq R \}$. For any $R$ such that $\min_{\|\theta\|_2 \leq R} F(\theta) < \min_{i} q_i \ell(0, y_i)$, $\theta_R$ is unique.

And if $\lim_{R \to \infty} \theta_R$ exists, then $\lim_{t \to \infty} \|\theta(t)\|_2$ also exists and the two limits are equal.

This result is an extension of Theorem 1 of (Ji et al., 2020). For the logistic loss, it is easy to show that it satisfies the conditions of the above theorem and $\lim_{R \to \infty} \theta_R = \hat{\theta}_{MM}$.

**Remark.** It is impossible to extend these results to wide neural networks like Theorem 4.4 because for a neural network, if $\|\theta(t)\|_2$ goes to infinity, then $\|\nabla_{\theta} f\|_2$ will also go to infinity. However, for a linear model, the gradient is a constant. Consequently, the gap between the neural networks and its linearized counterpart will “explode” under GD, so there can be no approximation theorem like Lemma 4.5 that can connect wide NNS to their linearized counterparts. Thus, we consider regularized GRW, for which $\|\theta(t)\|_2$ converges to a finite point and there is an approximation theorem.

5.2. Wide Neural Networks, with $L_2$ Regularization

Consider minimizing the regularized weighted empirical risk (15) with $\ell$ being the logistic loss. As in the regression
case, with $L_2$ regularization, GRW methods have different implicit biases than ERM for the same reasons as in Section 4.3. And similarly, we can show that in order for GRW methods to be sufficiently different from ERM, the regularization needs to be large enough to significantly lower the training performance. Specifically, in the following theorem we show that if the regularization is too small to lower the training performance, then a wide neural network trained with regularized GRW and the logistic loss will still be very close to the max-margin linearized neural network:

$$f_{\text{MM}}(x) = \langle \hat{\theta}_{\text{MM}}, \nabla_{\theta} f(x) \rangle$$

where

$$\hat{\theta}_{\text{MM}} = \arg \max_{\|\theta\|_2 = 1} \left\{ \min_{i=1, \ldots, n} y_i : \langle \theta, \nabla_{\theta} f(x_i) \rangle \right\}$$

(22)

Note that $f_{\text{MM}}$ does not depend on $q_i^{(t)}$. Moreover, using the result in the previous section we can show that a linearized neural network trained with unregularized ERM will converge to $f_{\text{MM}}$. The main result is the following:

**Theorem 5.3.** Suppose there exists $M_0 > 0$ such that $\|\nabla_{\theta} f(x)\|_2 \leq M_0$ for all test point $x$. For a wide NN satisfying Assumption 2, and for any GRW satisfying Assumption 1 with the logistic loss, if $d_1 = d_2 = \cdots = d_L = \bar{d}$ and $\nabla_{\theta} f(x_1), \ldots, \nabla_{\theta} f(x_n)$ are linearly independent and the learning rate is sufficiently small, then for any $\delta > 0$ there exists a constant $C > 0$ such that: with probability at least $(1 - \delta)$ over random initialization, as $\bar{d} \to \infty$, it holds that: for any $\epsilon \in (0, \frac{1}{4})$, if the empirical training error of the model satisfies

$$\limsup_{t \to \infty} \hat{R}(f^{(t)}_{\text{reg}}) < \epsilon$$

then for any test point $x$ such that $|f_{\text{MM}}(x)| > C \cdot (-\log 2\epsilon)^{-1/2}$, $f^{(t)}_{\text{reg}}(x)$ has the same sign as $f_{\text{MM}}(x)$ when $t$ is sufficiently large.

This result says that at any test point $x$ on which the max-margin linear classifier classifies with a margin of $O((-\log 2\epsilon)^{-1/2})$, the neural network has the same prediction. And as $\epsilon$ decreases, the confidence threshold also becomes lower. Similar to Theorem 4.6, this theorem provides the scaling of the gap between the regularized GRW model and the unregularized ERM model w.r.t. $\epsilon$.

The result in this section justifies the empirical observation in (Sagawa et al., 2020a) that by using large regularization, GRW can maintain a high worst-group test performance, with the cost of suffering a significant drop in training accuracy. On the other hand, if the regularization is small and the model can achieve nearly perfect training accuracy, then its worst-group test performance will still significantly drop.

### 6. Empirical Study

In this part, we empirically verify our theoretical findings.

**Figure 1.** Experimental results of ERM, importance weighting (IW) and Group DRO (GDRO) with the squared loss on six MNIST images with a linear model. All norms are $L_2$ norms.

**Figure 2.** Experimental results of ERM, importance weighting (IW) and Group DRO (GDRO) with $L_2$ regularization with the squared loss. Left two: $\mu = 0.1$; Right two: $\mu = 10$.

#### 6.1. MNIST Images

Towards verifying our results on linear models, we use 6 $28 \times 28$ MNIST images as training samples, 5 of them are digit 0 and 1 is digit 1. The group labels are the target labels as in learning with class imbalance, so there are 2 groups in total. The model is a 784-dimensional linear model. Here we only present the results for regression. Results for classification can be found in Appendix C.

We run ERM, importance weighting and Group DRO with the squared loss on this dataset from the same initial point with full-batch GD and no regularization for 5000 epochs (one iteration per epoch). The results are shown in Figure 1. The training loss of each method converges to 0, and the gap between the model weights of importance weighting (or Group DRO) and ERM converges to 0, meaning that all three model weights converge to the same point, whose $L_2$ norm is about 0.63. Figure 1d also shows that the group weights in Group DRO empirically satisfy Assumption 1.
Towards verifying our results on wide NN models, we converge to the same point. This shows that the regularization must be large enough to lower the training performance in order to make a significant difference to the implicit bias.

### 6.2. Waterbirds and CelebA

Towards verifying our results on wide NN models, we conduct experiments on two datasets, Waterbirds and CelebA, to investigate the effect of regularization in classification. Our empirical study extends that in (Sagawa et al., 2020a) that focuses on Group DRO; here we also include importance weighting, and more weight decay levels. For both datasets we use a ResNet-18 as the classifier. We run ERM, importance weighting (IW) and Group DRO under different levels of weight decay for 500 epochs on Waterbirds and 250 epochs on CelebA. Note that we do not strictly follow our $L_2$ penalty formulation (15), but we study the $L_2$ weight decay regularization most widely used in practice. The mean average training and worst-group test accuracies of the last 10 training epochs are reported in Table 1. To compare with early stopping, we also report the mean accuracies of epochs 11-20 with no regularization (blue entries). We do not apply weight decay to ERM because it does not affect ERM too much and is not our main focus.

On both datasets, early stopping achieves the best performances. Particularly, on Waterbirds, there is no clear sign that regularization could help prevent overfitting. When the regularization is small, the training accuracy is still 100% and the algorithm continues to overfit. However, when the regularization is large enough to lower the training accuracy, the worst-group test accuracy drops more because the model cannot learn the samples well under such a large regularization. Thus, perhaps not surprisingly, a lower training performance is only a necessary condition but not sufficient.

On CelebA, regularization does help mitigate overfitting, but a useful regularization (which makes the final performance close to the early stopping performance) must be large enough to lower the training accuracy. We also notice that Group DRO requires a smaller regularization than importance weighting: for importance weighting we need the weight decay level to be as large as 0.1 to achieve a similar performance as early stopping, but for Group DRO it only needs to be 0.03, and using 0.1 is actually harmful.

Overall, we find that using small regularization does not significantly improve the performance while using large regularization could result in training instability, as well as a loss in overall performance, and there may or may not be a small band for the regularization parameter where the worst-group test performance is better. This shows that regularization is not the universal way to improve GRW over ERM. Moreover, (Gulrajani & Lopez-Paz, 2021; Koh et al., 2021) showed that even with early stopping, GRW does not improve over ERM in real-world applications. Thus, we argue that it is important to study how to principally improve distributionally robust generalization.

### 7. Conclusion

In this work, we posit a broad class of what we call Generalized Reweighting (GRW) algorithms that include popular approaches such as importance weighting, and Distributionally Robust Optimization (DRO) variants, that were designed towards the task learning models that are robust to distributional shift. We show that when used to train overparameterized linear or wide NN models, even this very broad class of GRW algorithms does not improve over ERM, because they have the same implicit biases. We also showed that regularization does not help if it is not large enough to significantly lower the average training performance. Our results thus suggest to make progress towards learning models that are robust to distributional shift, we have to either go beyond this broad class of GRW algorithms, or design new losses specifically targeted to this class.

---

**Table 1.** Mean average accuracy (%) of the last 10 training epochs under different levels of weight decay (WD). Each entry is Average training accuracy / Worst-group test accuracy. Blue entries are mean accuracies of epochs 11-20 with no weight decay (early stopping). Each experiment is repeated five times with different random seeds and the 95% confidence intervals are reported.

| Dataset | WD     | ERM    | IW      | Group DRO |
|---------|--------|--------|---------|-----------|
|         | 0      | 100.0 ± 0.0/56.3 ± 1.8 | 100.0 ± 0.0/67.6 ± 1.1 | 100.0 ± 0.0/64.5 ± 1.6 |
|         | (11-20)| 95.1 ± 0.3/13.8 ± 2.8 | 92.4 ± 0.4/83.7 ± 0.6 | 92.9 ± 0.4/79.9 ± 2.1 |
| Waterbirds | 0.05   | 100.0 ± 0.0/71.0 ± 1.9 | 100.0 ± 0.0/63.5 ± 2.6 |           |
|         | 0.1    | 100.0 ± 0.0/67.7 ± 0.7 | 100.0 ± 0.0/54.7 ± 2.7 |           |
|         | 0.15   | 99.0 ± 0.7/53.7 ± 2.7 | 99.4 ± 0.6/52.5 ± 2.5 |           |
|         | 0.2    | 91.6 ± 2.0/35.9 ± 6.9 | 94.8 ± 0.9/38.0 ± 7.5 |           |
|         | (11-20)| 0      | 99.0 ± 0.2/40.2 ± 5.6 | 99.4 ± 0.1/42.7 ± 1.7 | 99.4 ± 0.1/49.5 ± 1.9 |
| CelebA  | 0.01   |         | 97.9 ± 0.2/50.0 ± 2.8 | 96.5 ± 0.5/67.2 ± 1.7 |
|         | 0.03   |         | 95.0 ± 0.2/62.8 ± 2.4 | **88.9 ± 1.1/83.1 ± 2.2** |
|         | 0.1    | **89.4 ± 2.0/76.0 ± 2.4** | 75.1 ± 9.5/50.6 ± 15.9 |           |

Understanding Why Generalized Reweighting Does Not Improve Over ERM
Understanding Why Generalized Reweighting Does Not Improve Over ERM

Codes

Codes for the MNIST images experiments are at https://colab.research.google.com/drive/1YtZMsAvOhZ0Rf0pFK1AjgSaG7WaVpFX5p?usp=sharing. Codes for the Waterbirds and CelebA experiments are at https://github.com/RuntianZ/grw-vs-erm.

Acknowledgements

We acknowledge the support of NSF via OAC-1934584, IIS-1909816, DARPA via HR00112020006, and ARL.

References

Allen-Zhu, Z., Li, Y., and Song, Z. A convergence theory for deep learning via over-parameterization. In International Conference on Machine Learning, pp. 242–252. PMLR, 2019.

Blodgett, S. L., Green, L., and O’Connor, B. Demographic dialectal variation in social media: A case study of African-American English. In Proceedings of the 2016 Conference on Empirical Methods in Natural Language Processing, pp. 1119–1130, Austin, Texas, November 2016. Association for Computational Linguistics. doi: 10.18653/v1/D16-1120.

Byrd, J. and Lipton, Z. What is the effect of importance weighting in deep learning? In Chaudhuri, K. and Salakhutdinov, R. (eds.), Proceedings of the 36th International Conference on Machine Learning, volume 97 of Proceedings of Machine Learning Research, pp. 872–881. PMLR, 09–15 Jun 2019.

Cao, K., Wei, C., Gaidon, A., Arechiga, N., and Ma, T. Learning imbalanced datasets with label-distribution-aware margin loss. Advances in Neural Information Processing Systems, 32:1567–1578, 2019.

Chizat, L., Oyallon, E., and Bach, F. On lazy training in differentiable programming. In Wallach, H., Larochelle, H., Beygelzimer, A., d’Alché-Buc, F., Fox, E., and Garnett, R. (eds.), Advances in Neural Information Processing Systems, volume 32. Curran Associates, Inc., 2019.

Du, S., Lee, J., Li, H., Wang, L., and Zhai, X. Gradient descent finds global minima of deep neural networks. In International Conference on Machine Learning, pp. 1675–1685. PMLR, 2019.

Duchi, J. and Namkoong, H. Learning models with uniform performance via distributionally robust optimization. arXiv preprint arXiv:1810.08750, 2018.

Dwork, C., Hardt, M., Pitassi, T., Reingold, O., and Zemel, R. Fairness through awareness. In Proceedings of the 3rd innovations in theoretical computer science conference, pp. 214–226, 2012.

Gulrajani, I. and Lopez-Paz, D. In search of lost domain generalization. In International Conference on Learning Representations, 2021.

Gunasekar, S., Lee, J., Soudry, D., and Srebro, N. Characterizing implicit bias in terms of optimization geometry. In Dy, J. and Krause, A. (eds.), Proceedings of the 35th International Conference on Machine Learning, volume 80 of Proceedings of Machine Learning Research, pp. 1832–1841. PMLR, 10–15 Jul 2018.

Hardt, M., Price, E., and Srebro, N. Equality of opportunity in supervised learning. In Lee, D., Sugiyama, M., Luxburg, U., Guyon, I., and Garnett, R. (eds.), Advances in Neural Information Processing Systems, volume 29, pp. 3315–3323. Curran Associates, Inc., 2016.

Hashimoto, T., Srivastava, M., Namkoong, H., and Liang, P. Fairness without demographics in repeated loss minimization. In Dy, J. and Krause, A. (eds.), International Conference on Machine Learning, volume 80 of Proceedings of Machine Learning Research, pp. 1929–1938, Stockholmsmässan, Stockholm Sweden, 10–15 Jul 2018. PMLR.

Hovy, D. and Søgaard, A. Tagging performance correlates with author age. In Proceedings of the 53rd annual meeting of the Association for Computational Linguistics and the 7th international joint conference on natural language processing (volume 2: Short papers), pp. 483–488, 2015.

Hu, W., Niu, G., Sato, I., and Sugiyama, M. Does distributionally robust supervised learning give robust classifiers? In International Conference on Machine Learning, pp. 2029–2037. PMLR, 2018.

Jacot, A., Gabriel, F., and Hongler, C. Neural tangent kernel: Convergence and generalization in neural networks. In Bengio, S., Wallach, H., Larochelle, H., Grauman, K., Cesa-Bianchi, N., and Garnett, R. (eds.), Advances in Neural Information Processing Systems, volume 31. Curran Associates, Inc., 2018.

Ji, Z., Dudík, M., Schapire, R. E., and Telgarsky, M. Gradient descent follows the regularization path for general losses. In Abernethy, J. and Agarwal, S. (eds.), Proceedings of Thirty Third Conference on Learning Theory, volume 125 of Proceedings of Machine Learning Research, pp. 2109–2136. PMLR, 09–12 Jul 2020.

Kini, G. R., Paraskevas, O., Oymak, S., and Thrampoulidis, C. Label-imbalanced and group-sensitive classification
under overparameterization. In Thirty-Fifth Conference on Neural Information Processing Systems, 2021.

Koh, P. W., Sagawa, S., Marklund, H., Xie, S. M., Zhang, M., Balsubramani, A., Hu, W., Yasunaga, M., Phillips, R. L., Gao, I., Lee, T., David, E., Stavness, I., Guo, W., Earnshaw, B., Haque, I., Beery, S. M., Leskovec, J., Kundaje, A., Pierson, E., Levine, S., Finn, C., and Liang, P. Wilds: A benchmark of in-the-wild distribution shifts. In Meila, M. and Zhang, T. (eds.), Proceedings of the 38th International Conference on Machine Learning, volume 139 of Proceedings of Machine Learning Research, pp. 5637–5664. PMLR, 18–24 Jul 2021.

Kusner, M. J., Loftus, J., Russell, C., and Silva, R. Counterfactual fairness. In Advances in neural information processing systems, pp. 4066–4076, 2017.

Lee, J., Xiao, L., Schoenholz, S., Bahri, Y., Novak, R., Sohl-Dickstein, J., and Pennington, J. Wide neural networks of any depth evolve as linear models under gradient descent. Advances in neural information processing systems, 32: 8572–8583, 2019.

Liu, E. Z., Haghgoo, B., Chen, A. S., Raghunathan, A., Koh, P. W., Sagawa, S., Liang, P., and Finn, C. Just train twice: Improving group robustness without training group information. In International Conference on Machine Learning, pp. 6781–6792. PMLR, 2021.

Menon, A. K., Jayasumana, S., Rawat, A. S., Jain, H., Veit, A., and Kumar, S. Long-tail learning via logit adjustment. In International Conference on Learning Representations, 2021.

Oren, Y., Sagawa, S., Hashimoto, T., and Liang, P. Distributionally robust language modeling. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP), pp. 4227–4237, Hong Kong, China, November 2019. Association for Computational Linguistics. doi: 10.18653/v1/D19-1432.

Rawls, J. Justice as fairness: A restatement. Harvard University Press, 2001.

Sagawa, S., Koh, P. W., Hashimoto, T. B., and Liang, P. Distributionally robust neural networks for group shifts: On the importance of regularization for worst-case generalization. In International Conference on Learning Representations, 2020a.

Sagawa, S., Raghunathan, A., Koh, P. W., and Liang, P. An investigation of why overparameterization exacerbates spurious correlations. In III, H. D. and Singh, A. (eds.), Proceedings of the 37th International Conference on Machine Learning, volume 119 of Proceedings of Machine Learning Research, pp. 8346–8356. PMLR, 13–18 Jul 2020b.

Shimodaira, H. Improving predictive inference under covariate shift by weighting the log-likelihood function. Journal of statistical planning and inference, 90(2):227–244, 2000.

Soudry, D., Hoffer, E., Nacson, M. S., Gunasekar, S., and Srebro, N. The implicit bias of gradient descent on separable data. The Journal of Machine Learning Research, 19(1):2822–2878, 2018.

Tatman, R. Gender and dialect bias in youtube’s automatic captions. In Proceedings of the First ACL Workshop on Ethics in Natural Language Processing, pp. 53–59, 2017.

Vershynin, R. Introduction to the non-asymptotic analysis of random matrices. arXiv preprint arXiv:1011.3027, 2010.

Wang, K. A., Chatterji, N. S., Haque, S., and Hashimoto, T. Is importance weighting incompatible with interpolating classifiers?, 2021.

Xu, D., Ye, Y., and Ruan, C. Understanding the role of importance weighting for deep learning. In International Conference on Learning Representations, 2021.

Xu, Z., Dan, C., Khim, J., and Ravikumar, P. Class-weighted classification: Trade-offs and robust approaches. In III, H. D. and Singh, A. (eds.), Proceedings of the 37th International Conference on Machine Learning, volume 119 of Proceedings of Machine Learning Research, pp. 10544–10554. PMLR, 13–18 Jul 2020.

Ye, H.-J., Chen, H.-Y., Zhan, D.-C., and Chao, W.-L. Identifying and compensating for feature deviation in imbalanced deep learning. arXiv preprint arXiv:2001.01385, 2020.

Zafar, M. B., Valera, I., Gomez Rodriguez, M., and Gummadi, K. P. Fairness beyond disparate treatment & disparate impact: Learning classification without disparate mistreatment. In Proceedings of the 26th international conference on world wide web, pp. 1171–1180, 2017.

Zemel, R., Wu, Y., Swersky, K., Pitassi, T., and Dwork, C. Learning fair representations. In International Conference on Machine Learning, pp. 325–333, 2013.

Zhai, R., Dan, C., Kolter, Z., and Ravikumar, P. Doro: Distributional and outlier robust optimization. In Meila, M. and Zhang, T. (eds.), Proceedings of the 38th International Conference on Machine Learning, volume 139 of Proceedings of Machine Learning Research, pp. 12345–12355. PMLR, 18–24 Jul 2021a.
Zhai, R., Dan, C., Suggala, A., Kolter, J. Z., and Ravikumar, P. K. Boosted CVaR classification. In Thirty-Fifth Conference on Neural Information Processing Systems, 2021b.
A. Related work

**Group Fairness.** Group fairness in machine learning was first studied in (Hardt et al., 2016) and (Zafar et al., 2017), where they required the model to perform equally well over all groups. Later, (Hashimoto et al., 2018) studied another type of group fairness called Rawlsian max-min fairness (Rawls, 2001), which does not require equal performance but rather requires high performance on the worst-off group. The subpopulation shift problem we study in this paper is most closely related to Rawlsian max-min fairness. A large body of recent work have studied how to improve this worst-group performance (Duchi & Namkoong, 2018; Oren et al., 2019; Liu et al., 2021; Zhai et al., 2021a). Recent work however observe that these approaches, when used with modern overparameterized models, easily overfit (Sagawa et al., 2020a; b). Apart from group fairness, there are also other notions of fairness, such as individual fairness (Dwork et al., 2012; Zemel et al., 2013) and counterfactual fairness (Kusner et al., 2017), which we do not study in this work.

**Implicit Bias Under the Overparameterized Setting.** For overparameterized models, there could be many model parameters which all minimize the training loss. In such cases, it is of interest to study the implicit bias of specific optimization algorithms such as gradient descent i.e. to what minimizer the model parameters will converge to (Du et al., 2019; Allen-Zhu et al., 2019). Our results use the NTK formulation of wide neural networks (Jacot et al., 2018), and specifically we use linearized neural networks to approximate such wide neural networks following (Lee et al., 2019). There is some criticism of this line of work, e.g. (Chizat et al., 2019) argued that infinitely wide neural networks fall in the “lazy training” regime and results might not be transferable to general neural networks. Nonetheless such wide neural networks are being widely studied in recent years, since they provide considerable insights into the behavior of more general neural networks, which are typically intractable to analyze otherwise.

B. Discussion

**B.1. Distributionally Robust Generalization**

A large body of prior work focused on improving distributionally robust optimization, but our results show that in many general cases in the interpolation regime, these methods do not improve over ERM on the test set. In other words, *distributionally robust optimization* does not necessarily have better *distributionally robust generalization* (DRG). Therefore, we argue that it is more important to study how to principally improve DRG, which is what people really want in the first place. Here we discuss two promising approaches to improving DRG in classification.

The first approach is *logit adjustment* (Menon et al., 2021), whose main purpose is to make a classifier have larger margins on smaller groups to improve its generalization on smaller groups. For example, (Cao et al., 2019) showed that in tasks with imbalanced classes, a classifier will have optimal DRG if the margin of class \( k \) is proportional to \( n_k^{-1/4} \) where \( n_k \) is the size of class \( k \) using standard generalization bounds. To achieve this, they added an \( O(n_k^{-1/4}) \) additive adjustment term to the logits outputted by the classifier. Following this spirit, (Menon et al., 2021) proposed the logit adjusted softmax cross-entropy loss (LA-loss) which also adds an additive adjustment term to the logits. (Ye et al., 2020) proposed the class-dependent temperature (CDT) which adds a multiplicative adjustment term to the logits by dividing the logits of different classes with different temperatures. (Kini et al., 2021) proposed to add both adjustment terms, and they designed a bi-level optimization framework where the lower level updates the model parameters and the upper level updates the parameters of the adjustment terms.

The second approach is changing the loss function. A recent paper (Wang et al., 2021) showed that for linear classifiers, one can change the implicit bias of GRW by replacing the exponentially-tailed logistic loss to the following polynomially-tailed loss:

\[
\ell_{\alpha, \beta}(\hat{y}, y) = \begin{cases} 
\ell_{\text{left}}(\hat{y}y), & \text{if } \hat{y}y < \beta \\
1/(|\hat{y}y - (\beta - 1)|^{\alpha}), & \text{if } \hat{y}y \geq \beta
\end{cases}
\]

(24)

And this result can be extended to GRW satisfying Assumption 1 using our Theorem 5.2. The reason why loss (24) works is that it changes \( \lim_{R \rightarrow \infty} \frac{\ell_{\text{left}}}{R} \).

There are many open questions about DRG. For example, is logit adjustment possible when the group labels are unknown

\footnote{The margin of a multi-class classifier is defined as follows: For a classifier \( f(x) \) that produces confidence scores, the margin over \((x, y)\) is \( f(x)_y - \max_{y' \neq y} f(x)_{y'} \), and the margin of a group is the smallest margin over any sample in that group.}
Understanding Why Generalized Reweighting Does Not Improve Over ERM during training? And what about regression? We believe that answering these fundamental questions is necessary for us to tackle difficult tasks in practice.

B.2. Does More Data Help?

Among the open questions is a very important one that involves the sample complexity of distributionally robust generalization. That is, does distributionally robust generalization require more data? It might seem quite natural that distributionally robust generalization could require more data than standard generalization. For instance, (Sagawa et al., 2020a) showed with experiments that when training under Group DRO without regularization and early stopping, as the training proceeds the model’s average performance would not change too much, but its worst-group performance would significantly drop, which implies that the model is much easier to overfit with respect to distributionally robust generalization than standard generalization. However, one caveat is that more data can sometimes even hurt distributional robustness, especially in the case where big groups grow even bigger. For example, (Sagawa et al., 2020b) made the surprising empirical observation that balancing the group sizes by removing lots of data from the majority groups and then training with ERM could achieve higher worst-group performance than using GRW on the original training set, though doing so wastes a huge amount of data. This implies that the extra large amount of data being removed actually hurts the distributional robustness.

In our results we proved that if the training set is small and fixed, then algorithms for distributional shift do not improve over ERM. With a larger training set, the performance could be different, but it does not mean that the performance would be improved. Therefore, while enlarging the training set with techniques like data augmentation or semi-supervised learning is in principle a good approach, be cautious that it does not always improve the distributional robustness, and we need to understand more deeply what extra data helps distributionally robust generalization and what hurts.

B.3. Extension to Multi-dimensional Regression / Multi-class Classification

In our results, we assume that $f : \mathbb{R}^d \rightarrow \mathbb{R}$ for simplicity, but our results can be very easily extended to the case where $f : \mathbb{R}^d \rightarrow \mathbb{R}^k$. For most of our results, the proof consists of two major components: (i) The linearized neural network will converge to some point (interpolator, max-margin classifier, etc.); (ii) The wide fully-connected neural network can be approximated by its linearized counterpart. For both components, the extension is very simple and straightforward. For (i), the proof only relies on the smoothness of the objective function and the upper quadratic bound it entails, and the function is still smooth when its output becomes multi-dimensional; For (ii), we can prove that $\sup_x \|f(x) - f_{\text{lin}}(x)\|_2 = O(d^{-1/4})$ in exactly the same way. Thus, all of our results hold for multi-dimensional regression and multi-class classification.

Particularly, for the multi-class cross-entropy loss, using Theorem 5.2 we can show that under any GRW satisfying Assumption 1, the direction of the weight of a linear classifier will converge to the following max-margin classifier:

$$\hat{\theta}_{\text{MM}} = \arg\min_{\theta} \left\{ \min_{i=1,\ldots,n} \left[ f(x_i)_{y_i} - \max_{y' \neq y_i} f(x_i)_{y'} \right] : \|\theta\|_2 = 1 \right\}$$

which is still independent of $q_i$.

B.4. Limitation

The major limitation of our results is that they are limited to the interpolation regime, i.e. the model converges to some interpolator or somewhere near an interpolator. The two main assumptions of our results are:

(i) The model is overparameterized, so that it can interpolate all training samples.

(ii) The model is trained for sufficiently long time, i.e. without early stopping.

Regarding (i), as mentioned earlier, (Chizat et al., 2019) argued that infinitely wide neural networks fall in the “lazy training” regime and results might not be transferable to general neural networks. However, this class of neural networks has been widely studied in recent years and has provided considerable insights into the behavior of general neural networks, which is hard to analyze otherwise.

Regarding (ii), in some easy tasks, when early stopping is applied, existing algorithms for distributional shift can do better than ERM (Sagawa et al., 2020a). However, as demonstrated in (Gulrajani & Lopez-Paz, 2021; Koh et al., 2021),
in real-world applications these methods still cannot significantly improve over ERM even with early stopping, so early stopping is not the universal solution towards this problem. Thus, even our results have this major limitation, we believe that they provide important insights into why existing methods do not improve over ERM, and they underscore the importance of a deeper understanding in distributionally robust generalization.

C. More Experiments

We run ERM, importance weighting and Group DRO on the synthetic dataset with 6 MNIST images as in Section 6.1 with the logistic loss and the polynomially-tailed loss (Eqn. (24), with $\alpha = 1$, $\beta = 0$ and $\ell_{\text{left}}$ being the logistic loss shifted to make the overall loss function continuous) on this dataset for 10 million epochs (note that we run for much more epochs because the convergence is very slow). The results are shown in Figure 3. From the plots we can see that:

- For either loss function, the training loss of each method converges to 0.

- In contrast to the theory that the norm of the ERM model will go to infinity and all models will converge to the max-margin classifier, the weight of the ERM model gets stuck at some point, and the norms of the gaps between the normalized model weights also get stuck. The reason is that the training loss has got so small that it becomes zero in the floating number representation, so the gradient also becomes zero and the training halts due to limited computational precision.

- However, we can still observe a fundamental difference between the logistic loss and the polynomially-tailed loss. For the logistic loss, the norm of the gap between importance weighting (or Group DRO) and ERM will converge to around 0.06 when the training stops, while for the polynomially-tailed loss, the norm will be larger than 0.22 and will keep growing, which shows that for the polynomially-tailed loss the normalized model weights do not converge to the same point.

- For either loss, the group weights of Group DRO still empirically satisfy Assumption 1.

D. Proofs

In this paper, for any matrix $A$, we will use $\|A\|_2$ to denote its spectral norm and $\|A\|_F$ to denote its Frobenius norm.
D.1. Background on Smoothness

A first-order differentiable function \( f \) over \( \mathcal{D} \) is called \( L \)-smooth for \( L > 0 \) if

\[
  f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} \| y - x \|^2 \quad \forall x, y \in \mathcal{D}
\]

which is also called the upper quadratic bound. If \( f \) is second-order differentiable and \( \mathcal{D} \) is a convex set, then \( f \) is \( L \)-smooth is equivalent to

\[
  v^\top \nabla^2 f(x)v \leq L \quad \forall \|v\|_2 = 1, \forall x \in \mathcal{D}
\]

A classical result in convex optimization is the following:

**Theorem D.1.** If \( f(x) \) is convex and \( L \)-smooth with a unique finite minimizer \( x^\star \), and is minimized by gradient descent \( x_{t+1} = x_t - \eta \nabla f(x_t) \) starting from \( x_0 \) where the learning rate \( \eta \leq \frac{1}{L} \), then we have

\[
  f(x_T) \leq f(x^\star) + \frac{1}{\eta T} \| x_0 - x^\star \|^2_2
\]

which also implies that \( x_T \) converges to \( x^\star \) as \( T \to \infty \).

D.2. Proofs for Subsection 4.1

D.2.1. Proof of Theorem 4.1

Using the key intuition, the weight update rule (2) implies that \( \theta^{(t+1)} - \theta^{(t)} \in \text{span}\{x_1, \ldots, x_n\} \) for all \( t \), which further implies that \( \theta^{(t)} - \theta^{(0)} \in \text{span}\{x_1, \ldots, x_n\} \) for all \( t \). By Cramer’s rule, in this \( \theta \)-dimensional subspace there exists only one \( \theta^* \) such that \( \theta^* - \theta^{(0)} \in \text{span}\{x_1, \ldots, x_n\} \) and \( \langle \theta^*, x_i \rangle \) for all \( i \). Then we have

\[
  \| X^\top (\theta^{(t)} - \theta^*) \|_2 = \| (X^\top \theta^{(t)} - Y) - (X^\top \theta^* - Y) \|_2 \leq \| X^\top \theta^{(t)} - Y \|_2 + \| X^\top \theta^* - Y \|_2 \to 0
\]

because \( \| X^\top \theta - Y \|_2 = 2\sqrt{R(f(x; \theta))} \). On the other hand, let \( s_{\text{min}} \) be the smallest singular value of \( X \). Since \( X \) is full-rank, \( s_{\text{min}} > 0 \), and \( \| X^\top (\theta^{(t)} - \theta^*) \|_2 \geq s_{\text{min}} \| \theta^{(t)} - \theta^* \|_2 \). This shows that \( \| \theta^{(t)} - \theta^* \|_2 \to 0 \). Thus, \( \theta^{(t)} \) converges to this unique \( \theta^* \).

D.2.2. Proof of Theorem 4.2

To help our readers understand the proof more easily, we will first prove the result for static GRW where \( q_i^{(t)} = q_i \) for all \( t \), and then we will prove the result for dynamic GRW that satisfy \( q_i^{(t)} \to q_i \) as \( t \to \infty \).

**Static GRW.** We first prove the result for all static GRW such that \( \min_i q_i = q^* > 0 \).

We will use smoothness introduce in Appendix D.1. Denote \( A = \sum_{i=1}^n \| x_i \|^2_2 \). The empirical risk of the linear model \( f(x) = \langle \theta, x \rangle \) is

\[
  F(\theta) = \sum_{i=1}^n q_i (\theta_i^\top x_i - y_i)^2
\]

whose Hessian is

\[
  \nabla^2_{\theta} F(\theta) = 2 \sum_{i=1}^n q_i x_i x_i^\top
\]

So for any unit vector \( v \in \mathbb{R}^d \), we have (since \( q_i \in [0, 1] \))

\[
  v^\top \nabla^2_{\theta} F(\theta)v = 2 \sum_{i=1}^n q_i (x_i^\top v)^2 \leq 2 \sum_{i=1}^n q_i \| x_i \|^2_2 \leq 2A
\]

which implies that \( F(\theta) \) is \( 2A \)-smooth. Thus, we have the following upper quadratic bound: for any \( \theta_1, \theta_2 \in \mathbb{R}^d \),

\[
  F(\theta_2) \leq F(\theta_1) + \langle \nabla_{\theta} F(\theta_1), \theta_2 - \theta_1 \rangle + A \| \theta_2 - \theta_1 \|^2_2
\]
We still denote $g(\theta(t)) = \langle X^\top \theta(t) - Y \rangle \in \mathbb{R}^n$. We can see that $\|\sqrt{Q}g(\theta(t))\|_2 = F(\theta(t))$, where $\sqrt{Q} = \text{diag}(\sqrt{q_1}, \cdots, \sqrt{q_n})$. Thus, $\nabla F(\theta(t)) = 2XQg(\theta(t))$. The update rule of a static GRW with gradient descent and the squared loss is:

$$\theta(t+1) = \theta(t) - \eta \sum_{i=1}^{n} q_i x_i (f(t)(x_i) - y_i) = \theta(t) - \eta XQg(\theta(t))$$

(34)

Substituting $\theta_1$ and $\theta_2$ in (33) with $\theta(t)$ and $\theta(t+1)$ yields

$$F(\theta(t+1)) \leq F(\theta(t)) - 2\eta g(\theta(t))^\top Q^\top XQg(\theta(t)) + A \left\| \eta XQg(\theta(t)) \right\|_2^2$$

(35)

Since $x_1, \cdots, x_n$ are linearly independent, $X^\top X$ is a positive definite matrix. Denote the smallest eigenvalue of $X^\top X$ by $\lambda_{\min} > 0$. And $\|Qg(\theta(t))\|_2 \geq \sqrt{q^*} \|g(\theta(t))\|_2 = \sqrt{q^*} F(\theta(t))$, so we have $g(\theta(t))^\top Q^\top XQg(\theta(t)) \geq q^* \lambda_{\min} F(\theta(t))$. Thus,

$$F(\theta(t+1)) \leq F(\theta(t)) - 2\eta q^* \lambda_{\min} F(\theta(t)) + A \eta^2 \|X\sqrt{Q}\|_2^2 \|Qg(\theta(t))\|_2^2$$

$$\leq F(\theta(t)) - 2\eta q^* \lambda_{\min} F(\theta(t)) + A \eta^2 \|X\sqrt{Q}\|_F^2 F(\theta(t))$$

$$\leq F(\theta(t)) - 2\eta q^* \lambda_{\min} F(\theta(t)) + A \eta^2 \|X\|_F^2 F(\theta(t))$$

$$= (1 - 2\eta q^* \lambda_{\min} + A^2 \eta^2) F(\theta(t))$$

(36)

Let $\eta_0 = \frac{q^* \lambda_{\min}}{A^2}$. For any $\eta \leq \eta_0$, we have $F(\theta(t+1)) \leq (1 - \eta q^* \lambda_{\min}) F(\theta(t))$ for all $t$, which implies that $\lim_{t \to \infty} F(\theta(t)) = 0$. This implies that the empirical training risk must converge to 0.

**Dynamic GRW.** Now we prove the result for all dynamic GRW satisfying Assumption 1. By Assumption 1, for any $\epsilon > 0$, there exists $t_\epsilon$ such that for all $t \geq t_\epsilon$ and all $i$,

$$q_i(t) \in (q_i - \epsilon, q_i + \epsilon)$$

(37)

This is because for all $i$, there exists $t_i$ such that for all $t \geq t_i$, $q_i(t) \in (q_i - \epsilon, q_i + \epsilon)$. Then, we can define $t_\epsilon = \max\{t_1, \cdots, t_n\}$. Denote the largest and smallest eigenvalues of $X^\top X$ by $\lambda_{\max}$ and $\lambda_{\min}$, and because $X$ is full-rank, we have $\lambda_{\min} > 0$. Define $\epsilon = \min\{\frac{q^* \lambda_{\min}}{\sqrt{2}}, \frac{q^* \lambda_{\min}^2}{\lambda_{\max}}\}$, and then $t_\epsilon$ is also fixed.

We still denote $Q = \text{diag}(q_1, \cdots, q_n)$. When $t \geq t_\epsilon$, the update rule of a dynamic GRW with gradient descent and the squared loss is:

$$\theta(t+1) = \theta(t) - \eta XQ_\epsilon(t)(X^\top \theta(t) - Y)$$

(38)

where $Q_\epsilon(t) = Q(t)$, and we use the subscript $\epsilon$ to indicate that $\|Q_\epsilon(t) - Q\|_2 < \epsilon$. Then, note that we can rewrite $Q_\epsilon(t)$ as $Q_\epsilon(t) = \sqrt{Q_{3\epsilon}(t)} \cdot \sqrt{Q}$ as long as $\epsilon \leq q^* / 3$. This is because $q_i + \epsilon \leq \sqrt{(q_i + 3\epsilon)q_i}$ and $q_i - \epsilon \geq \sqrt{(q_i - 3\epsilon)q_i}$ for all $\epsilon \leq q_i / 3$, and $q_i \geq q^*$. Thus, we have

$$\theta(t+1) = \theta(t) - \eta X\sqrt{Q_{3\epsilon}(t)} \sqrt{Q}g(\theta(t)) \text{ where } Q_{3\epsilon}(t) = \sqrt{Q_{3\epsilon}(t)} \cdot \sqrt{Q}$$

(39)

Again, substituting $\theta_1$ and $\theta_2$ in (33) with $\theta(t)$ and $\theta(t+1)$ yields

$$F(\theta(t+1)) \leq F(\theta(t)) - 2\eta g(\theta(t))^\top Q^\top XQ\sqrt{Q_{3\epsilon}(t)} \sqrt{Q}g(\theta(t)) + A \left\| \eta X\sqrt{Q_{3\epsilon}(t)} \sqrt{Q}g(\theta(t)) \right\|_2^2$$

(40)
Then, note that
\[
\begin{align*}
|g(\theta^{(i)})^T Q^T X^T X \left( \sqrt{Q_{3e}^{(i)}} - \sqrt{Q} \right) \sqrt{Q} g(\theta^{(i)})| \\
\leq \left\| \sqrt{Q}^T X^T X \left( \sqrt{Q_{3e}^{(i)}} - \sqrt{Q} \right) \right\|_2 \left\| \sqrt{Q} g(\theta^{(i)}) \right\|_2^2 \\
\leq \left\| Q \right\|_2 \left\| X^T X \right\|_2 \left\| \sqrt{Q_{3e}^{(i)}} - \sqrt{Q} \right\|_2 \left\| \sqrt{Q} g(\theta^{(i)}) \right\|_2^2 \leq \lambda_{\text{max}}^{\max} \sqrt{3} \epsilon F(\theta^{(i)})
\end{align*}
\]  
where the last step comes from the following fact: for all \( \epsilon < q_i/3 \),
\[
\sqrt{q_i + 3\epsilon} - \sqrt{3\epsilon} \leq \sqrt{3\epsilon} \quad \text{and} \quad \sqrt{q_i} - \sqrt{q_i - 3\epsilon} \leq \sqrt{3\epsilon}
\]  
And as proved before, we also have
\[
g(\theta^{(i)})^T Q^T X^T X Q g(\theta^{(i)}) \geq q^* \lambda_{\text{min}} F(\theta^{(i)})
\]  
Since \( \epsilon \leq \frac{(q^* \lambda_{\text{min}}^2)}{12 \lambda_{\text{max}}^2} \), we have
\[
g(\theta^{(i)})^T Q^T X^T X \sqrt{Q_{3e}^{(i)}} \sqrt{Q} g(\theta^{(i)}) \geq \left( q^* \lambda_{\text{min}} - \lambda_{\text{max}} \sqrt{3\epsilon} \right) F(\theta^{(i)}) \geq \frac{1}{2} q^* \lambda_{\text{min}} F(\theta^{(i)})
\]  
Thus,
\[
F(\theta^{(t+1)}) \leq F(\theta^{(t)}) - \eta q^* \lambda_{\text{min}} F(\theta^{(t)}) + A\eta^2 \left\| X \sqrt{Q_{3e}^{(t)}} \right\|_2 \left\| \sqrt{Q} g(\theta^{(t)}) \right\|_2^2 \\
\leq (1 - \eta q^* \lambda_{\text{min}} + A^2 \eta^2 (1 + 3\epsilon)) F(\theta^{(t)}) \\
\leq (1 - \eta q^* \lambda_{\text{min}} + 2A^2 \eta^2) F(\theta^{(t)})
\]  
for all \( \epsilon \leq 1/3 \). Let \( \eta_0 = \frac{q^* \lambda_{\text{min}}}{4A^2} \). For any \( \eta \leq \eta_0 \), we have \( F(\theta^{(t+1)}) \leq (1 - \eta q^* \lambda_{\text{min}}/2) F(\theta^{(t)}) \) for all \( t \geq t_\epsilon \), which implies that \( \lim_{t \to \infty} F(\theta^{(t)}) = 0 \). Thus, the empirical training risk converges to 0. \( \square \)

**D.3. Proofs for Subsection 4.2**

**D.3.1. PROOF OF LEMMA 4.3**

Note that the first \( l \) layers (except the output layer) of the original NTK formulation and our new formulation are the same, so we still have the following proposition:

**Proposition D.2** (Proposition 1 in (Jacot et al., 2018)). If \( \sigma \) is Lipschitz and \( d_l \to \infty \) for \( l = 1, \cdots, L \) sequentially, then for all \( l = 1, \cdots, L \), the distribution of a single element of \( h_l \) converges in probability to a zero-mean Gaussian Process of covariance \( \Sigma^l \) that is defined recursively by:
\[
\begin{align*}
\Sigma^1(x, x') &= \frac{1}{d_0} x^\top x' + \beta^2 \\
\Sigma^l(x, x') &= \mathbb{E}_f [\sigma(f(x))\sigma(f(x'))] + \beta^2
\end{align*}
\]
where \( f \) is sampled from a zero-mean Gaussian process of covariance \( \Sigma^{l-1} \).

Now we show that for an infinitely wide neural network with \( L \geq 1 \) hidden layers, \( \Theta^{(0)} \) converges in probability to the following non-degenerated deterministic limiting kernel
\[
\Theta = \mathbb{E}_{f \sim \Sigma^L} [\sigma(f(x))\sigma(f(x'))] + \beta^2
\]  
Consider the output layer \( h^{L+1} = \frac{W_L}{\sqrt{d}} \sigma(h^L) + \beta b^L \). We can see that for any parameter \( \theta \), before the output layer,
\[
\nabla_{\theta} h^{L+1} = \text{diag}(\sigma(h^L)) \frac{W_L}{\sqrt{d_L}} \nabla_{\theta} h^L = 0
\]
And for $W^L$ and $b^L$, we have
\[
\nabla_W h^{L+1} = \frac{1}{\sqrt{d_L}} \sigma(h^L) \quad \text{and} \quad \nabla_b h^{L+1} = \beta
\] (49)

Then we can achieve (47) by the law of large numbers.

**D.3.2. PROOF OF LEMMA 4.5**

We will use the following short-hand in the proof:
\[
\begin{align*}
&g(\theta^{(t)}) = f^{(t)}(X) - Y \\
&J(\theta^{(t)}) = \nabla_\theta f(X; \theta^{(t)}) \in \mathbb{R}^{p \times n} \\
&\Theta^{(t)} = J(\theta^{(t)})^\top J(\theta^{(t)})
\end{align*}
\] (50)

For any $\epsilon > 0$, there exists $t_\epsilon$ such that for all $t \geq t_\epsilon$ and all $i, q_i^{(t)} \in (q_i - \epsilon, q_i + \epsilon)$. Like what we have done in (39), we can rewrite $Q^{(t)} = Q_{\epsilon}^{(t)} = \sqrt{Q_{3\epsilon}^{(t)}} \cdot \sqrt{Q}$, where $Q = \text{diag}(q_1, \ldots, q_n)$.

The update rule of a GRW with gradient descent and the squared loss for the wide neural network is:
\[
\theta^{(t+1)} = \theta^{(t)} - \eta J(\theta^{(t)}) Q^{(t)} g(\theta^{(t)})
\] (51)

and for $t \geq t_\epsilon$, it can be rewritten as
\[
\theta^{(t+1)} = \theta^{(t)} - \eta J(\theta^{(t)}) \sqrt{Q_{3\epsilon}^{(t)}} \left[ \sqrt{Q} g(\theta^{(t)}) \right]
\] (52)

First, we will prove the following theorem:

**Theorem D.3.** There exist constants $M > 0$ and $\epsilon_0 > 0$ such that for all $\epsilon \in (0, \epsilon_0]$, $\eta \leq \eta^*$ and any $\delta > 0$, there exist $R_0 > 0$, $\bar{D} > 0$ and $B > 1$ such that for any $\bar{d} \geq \bar{D}$, the following (i) and (ii) hold with probability at least $(1 - \delta)$ over random initialization when applying gradient descent with learning rate $\eta$:

(i) For all $t \leq t_\epsilon$, there is
\[
\left\| g(\theta^{(t)}) \right\|_2 \leq B^t R_0
\] (53)

\[
\sum_{j=1}^{t} \left\| \theta^{(j)} - \theta^{(j-1)} \right\|_2 \leq \eta M R_0 \sum_{j=1}^{t} B^{j-1} < \frac{MB^t R_0}{B - 1}
\] (54)

(ii) For all $t \geq t_\epsilon$, we have
\[
\left\| \sqrt{Q} g(\theta^{(t)}) \right\|_2 \leq \left( 1 - \frac{\eta q^* \lambda_{\min}}{3} \right)^{t-t_\epsilon} B^t R_0
\] (55)

\[
\sum_{j=t_\epsilon+1}^{t} \left\| \theta^{(j)} - \theta^{(j-1)} \right\|_2 \leq \eta \sqrt{1 + 3\epsilon MB^{t_\epsilon} R_0} \sum_{j=t_\epsilon+1}^{t} \left( 1 - \frac{\eta q^* \lambda_{\min}}{3} \right)^{j-t_\epsilon}
\] (56)

\[
< \frac{3\sqrt{1 + 3\epsilon MB^{t_\epsilon} R_0}}{q^* \lambda_{\min}}
\]

**Proof.** The proof is based on the following lemma:

**Lemma D.4** (Local Lipschitzness of the Jacobian). Under Assumption 2, there is a constant $M > 0$ such that for any $C_0 > 0$ and any $\delta > 0$, there exists a $\bar{D}$ such that: If $\bar{d} \geq \bar{D}$, then with probability at least $(1 - \delta)$ over random initialization,
for any $x$ such that $\|x\|_2 \leq 1$,
\[
\begin{cases}
\|\nabla_\theta f(x; \theta) - \nabla_\theta f(x; \tilde{\theta})\|_2 \leq \frac{M}{\sqrt{d}} \|\theta - \tilde{\theta}\|_2 \\
\|\nabla_\theta f(x; \theta)\|_2 \leq M \\
\|J(\theta) - J(\tilde{\theta})\|_F \leq \frac{M}{\sqrt{d}} \|\theta - \tilde{\theta}\|_2, \\
\|J(\theta)\|_F \leq M
\end{cases}
\] (57)

where $B(\theta(0), R) = \{\theta : \|\theta - \theta(0)\|_2 < R\}$.

The proof of this lemma can be found in Appendix D.3.3. Note that for any $x$, $f^{(0)}(x) = \beta b^L$ where $b^L$ is sampled from the standard Gaussian distribution. Thus, for any $\delta > 0$, there exists a constant $R_0$ such that with probability at least $(1 - \delta/3)$ over random initialization,
\[
\|g(\theta(0))\|_2 < R_0
\] (58)

And by Proposition 4.3, there exists $D_2 \geq 0$ such that for any $\hat{d} \geq D_2$, with probability at least $(1 - \delta/3)$,
\[
\|\Theta - \Theta(0)\|_F \leq \frac{q^* \lambda_{\min}}{3}
\] (59)

Let $M$ be the constant in Lemma D.4. Let $\epsilon_0 = \frac{(Q^* \lambda_{\min})^2}{10BM}$. Let $B = 1 + \eta^* M^2$, and $C_0 = \frac{MB^t R_0}{B-1} + 3\sqrt{1+\frac{M}{q^* \lambda_{\min}}} B^t R_0$.

By Lemma D.4, there exists $D_1 > 0$ such that with probability at least $(1 - \delta/3)$, for any $\hat{d} \geq D_1$, (57) is true for all $\theta, \tilde{\theta} \in B(\theta(0), C_0)$.

By union bound, with probability at least $(1 - \delta)$, (57), (58) and (59) are all true. Now we assume that all of them are true, and prove (53) and (54) by induction. (53) is true for $t = 0$ due to (58), and (54) is always true for $t = 0$. Suppose (53) and (54) are true for $t$, then for $t + 1$ we have
\[
\|\theta^{(t+1)} - \tilde{\theta}^{(t)}\|_2 \leq \eta \|J(\tilde{\theta}^{(t)})Q^{(t)}\|_2 \|g(\tilde{\theta}^{(t)})\|_2 \leq \eta \|J(\theta^{(t)})Q^{(t)}\|_F \|g(\theta^{(t)})\|_2 \leq \eta \|J(\theta^{(t)})\|_F \|g(\theta^{(t)})\|_2 \leq M\eta B^t R_0
\] (60)

So (54) is also true for $t + 1$. And we also have
\[
\|g(\theta^{(t+1)})\|_2 = \|g(\tilde{\theta}^{(t+1)} - g(\theta^{(t)})) + g(\tilde{\theta}^{(t)})\|_2 \\
= \|J(\tilde{\theta}^{(t)})^\top (\theta^{(t+1)} - \theta^{(t)}) + g(\tilde{\theta}^{(t)})\|_2 \\
= \|\eta J(\tilde{\theta}^{(t)})^\top J(\theta^{(t)})Q^{(t)}g(\tilde{\theta}^{(t)}) + g(\tilde{\theta}^{(t)})\|_2 \\
\leq \|I - \eta J(\tilde{\theta}^{(t)})^\top J(\theta^{(t)})Q^{(t)}\|_2 \|g(\tilde{\theta}^{(t)})\|_2 \leq \left(1 + \|\eta J(\tilde{\theta}^{(t)})^\top J(\theta^{(t)})Q^{(t)}\|_2\right) \|g(\tilde{\theta}^{(t)})\|_2 \leq \left(1 + \|J(\tilde{\theta}^{(t)})\|_F \|J(\theta^{(t)})\|_F\right) \|g(\tilde{\theta}^{(t)})\|_2 \leq \|g(\tilde{\theta}^{(t)})\|_2 \leq B^{t+1} R_0
\] (61)

Therefore, (53) and (54) are true for all $t \leq t_*$, which implies that $\|\sqrt{Q} g(\tilde{\theta}^{(t)})\|_2 \leq \|g(\tilde{\theta}^{(t)})\|_2 \leq B^t R_0$, so (55) is true for $t = t_*$. And (56) is obviously true for $t = t_*$. Now, let us prove (ii) by induction. Note that when $t \geq t_*$, we have the alternative update rule (52). If (55) and (56) are true for $t$, then for $t + 1$, there is
where $\tilde{\theta}^{(t)}$ is some linear interpolation between $\theta^{(t)}$ and $\theta^{(t+1)}$. Now we prove that

$$\left\| I - \eta \sqrt{Q} J (\tilde{\theta}^{(t)})^\top J (\theta^{(t)}) \sqrt{Q_{3e}} \right\|_2 \leq 1 - \frac{\eta q^* \lambda_{\min}^*}{3}$$

(64)

For any unit vector $v \in \mathbb{R}^n$, we have

$$v^\top (I - \eta \sqrt{Q} \Theta \sqrt{Q}) v = 1 - \eta v^\top \sqrt{Q} \Theta \sqrt{Q} v$$

(65)

$$\left\| \sqrt{Q} v \right\|_2 \leq \sqrt{q^*},$$

so for any $\eta \leq \eta^*$, $v^\top (I - \eta \sqrt{Q} \Theta \sqrt{Q}) v \in [0, 1 - \eta \lambda_{\min}^* q^*]$, which implies that $\left\| I - \eta \sqrt{Q} \Theta \sqrt{Q} \right\|_2 \leq 1 - \eta \lambda_{\min}^* q^*$. Thus,

$$\left\| I - \eta \sqrt{Q} J (\tilde{\theta}^{(t)})^\top J (\theta^{(t)}) \sqrt{Q_{3e}} \right\|_2 \leq 1 - \eta \lambda_{\min}^* q^* + \eta \left\| \sqrt{Q} (\Theta - \Theta^{(0)}) \sqrt{Q} \right\|_F + \eta \left\| \sqrt{Q} (J (\theta^{(0)})^\top J (\theta^{(0)}) - J (\tilde{\theta}^{(t)})^\top J (\theta^{(t)})) \sqrt{Q} \right\|_F$$

(66)

$$\leq 1 - \eta \lambda_{\min}^* q^* + \frac{\eta \lambda_{\min}^* q^*}{3} + \frac{\eta M^2}{\sqrt{d}} \left( \left\| \theta^{(t)} - \theta^{(0)} \right\|_2 + \left\| \tilde{\theta}^{(t)} - \theta^{(0)} \right\|_2 \right) \leq 1 - \frac{\eta q^* \lambda_{\min}^*}{2}$$

for all $d \geq \max \{ D_1, D_2, \left( \frac{12 M^2 C_2}{\eta^* \lambda_{\min}^*} \right)^4 \}$, which implies that

$$\left\| I - \eta \sqrt{Q} J (\tilde{\theta}^{(t)})^\top J (\theta^{(t)}) \sqrt{Q_{3e}} \right\|_2 \leq 1 - \frac{\eta q^* \lambda_{\min}^*}{2} + \eta \sqrt{Q} J (\tilde{\theta}^{(t)})^\top J (\theta^{(t)}) \left( \sqrt{Q_{3e}} - \sqrt{Q} \right) \right\|_2$$

(67)

$$\leq 1 - \frac{\eta q^* \lambda_{\min}^*}{2} + \eta M^2 \sqrt{3} \epsilon \leq 1 - \frac{\eta q^* \lambda_{\min}^*}{3}$$

(due to (42))
then we have so it follows that

\[
\theta \sim \mathcal{N}(\mu, \Sigma)
\]

Returning back to the proof of Lemma 4.5. Choose and fix an \( \epsilon \) such that \( \epsilon < \min \{ \epsilon_0, \frac{1}{3} \left( \frac{q^*\lambda_{\min}}{\max(q^*, \lambda_{\min})} \right)^2 \} \), where \( \epsilon_0 \) is defined by Theorem D.3. Then, \( t_* \) is also fixed. There exists \( \tilde{D} \geq 0 \) such that for any \( \tilde{d} \geq \tilde{D} \), with probability at least \( 1 - \delta \), Theorem D.3 and Lemma D.4 are true and

\[
\left\| \Theta - \Theta^{(0)} \right\|_F \leq \frac{q^*\lambda_{\min}}{3}
\]

which immediately implies that

\[
\left\| \Theta^{(0)} \right\|_2 \leq \left\| \Theta \right\|_2 + \left\| \Theta - \Theta^{(0)} \right\|_F \leq \lambda_{\max} + \frac{q^*\lambda_{\min}}{3}
\]

We still denote \( B = 1 + \eta^*M^2 \) and \( C_0 = \frac{MB^*R_0}{B-1} + \frac{3\sqrt{1+\epsilon\epsilon\epsilon}MB^*R_0}{q^*\lambda_{\min}} \). Theorem D.3 ensures that for all \( t, \theta^{(t)} \in B(\theta^{(0)}, C_0) \).

Then we have

\[
\left\| I - \eta\sqrt{Q}\Theta^{(0)}\sqrt{Q} \right\|_2 \leq \left\| I - \eta\sqrt{Q}\Theta\sqrt{Q} \right\|_2 + \left\| \sqrt{Q}(\Theta - \Theta^{(0)})\sqrt{Q} \right\|_2
\]

\[
\leq 1 - \frac{q^*\lambda_{\min}}{3} + \frac{\eta\lambda_{\max} + \frac{\eta^*\lambda_{\min}}{3}}{3} = 1 - \frac{2q^*\lambda_{\min}}{3}
\]

so it follows that

\[
\left\| I - \eta\sqrt{Q}\Theta^{(0)}\sqrt{Q} \right\|_2 \leq \left\| I - \eta\sqrt{Q}\Theta^{(0)}\sqrt{Q} \right\|_2 + \left\| \sqrt{Q}(\Theta^{(0)} - \sqrt{Q}) \right\|_2
\]

Thus, for all \( \epsilon < \frac{1}{3} \left( \frac{q^*\lambda_{\min}}{\max(q^*, \lambda_{\min})} \right)^2 \), there is

\[
\left\| I - \eta\sqrt{Q}\Theta^{(0)}\sqrt{Q} \right\|_2 \leq 1 - \frac{\eta q^*\lambda_{\min}}{3}
\]

The update rule of the GRW for the linearized neural network is:

\[
\theta_{\text{lin}}^{(t+1)} = \theta_{\text{lin}}^{(t)} - \eta J(\theta^{(t)})Q^{(t)}g_{\text{lin}}(\theta^{(t)})
\]

where we use the subscript “lin” to denote the linearized neural network, and with a slight abuse of notion denote \( g_{\text{lin}}(\theta^{(t)}) = g(\theta_{\text{lin}}^{(t)}) \).

First, let us consider the training data \( X \). Denote \( \Delta_t = g_{\text{lin}}(\theta^{(t)}) - g(\theta^{(t)}) \). We have

\[
\begin{cases}
\begin{aligned}
g_{\text{lin}}(\theta^{(t+1)}) - g_{\text{lin}}(\theta^{(t)}) &= -\eta J(\theta^{(t)})^T J(\theta^{(0)})Q^{(t)}g_{\text{lin}}(\theta^{(t)}) \\
g(\theta^{(t+1)}) - g(\theta^{(t)}) &= -\eta J(\theta^{(t)})^T J(\theta^{(0)})Q^{(t)}g(\theta^{(t)})
\end{aligned}
\end{cases}
\]

where \( \tilde{\theta}^{(t)} \) is some linear interpolation between \( \theta^{(t)} \) and \( \theta^{(t+1)} \). Thus,

\[
\Delta_{t+1} - \Delta_t = \eta \left[ J(\tilde{\theta}^{(t)})^T J(\theta^{(t)}) - J(\theta^{(0)})^T J(\theta^{(0)}) \right] Q^{(t)}g(\theta^{(t)})
\]

By Lemma D.4, we have

\[
\left\| J(\tilde{\theta}^{(t)})^T J(\theta^{(t)}) - J(\theta^{(0)})^T J(\theta^{(0)}) \right\|_F \leq \left\| J(\tilde{\theta}^{(t)}) - J(\theta^{(0)}) \right\|_F + \left\| J(\theta^{(0)})^T (J(\theta^{(t)}) - J(\theta^{(0)}) \right\|_F \leq 2M^2C_0\tilde{d}^{-1/4}
\]
which implies that for all $t < t_\epsilon$,
\[
\|\Delta_{t+1}\|_2 \leq \left\| I - \eta J(\theta^{(0)})^\top J(\theta^{(0)}) Q^{(t)} \right\|_F \| \Delta_t \|_2 + \| \eta \left[ J(\theta^{(t)})^\top J(\theta^{(0)}) - J(\theta^{(0)})^\top J(\theta^{(0)}) \right] Q^{(t)} g(\theta^{(t)}) \|_2 \\
\leq \left\| I - \eta J(\theta^{(0)})^\top J(\theta^{(0)}) Q^{(t)} \right\|_F \| \Delta_t \|_2 + \| \eta \left[ J(\theta^{(t)})^\top J(\theta^{(t)}) - J(\theta^{(0)})^\top J(\theta^{(0)}) \right] \|_F \| g(\theta^{(t)}) \|_2 \\
\leq (1 + \eta M^2) \| \Delta_t \|_2 + 2\eta M^2 C_0 B^t R_0 \tilde{d}^{-1/4} \\
\leq B \| \Delta_t \|_2 + 2\eta M^2 C_0 B^t R_0 \tilde{d}^{-1/4}
\]

Therefore, we have
\[
B^{- (t+1)} \| \Delta_{t+1} \|_2 \leq B^{- t} \| \Delta_t \|_2 + 2\eta M^2 C_0 B^{t-1} R_0 \tilde{d}^{-1/4}
\]

Since $\Delta_0 = 0$, it follows that for all $t \leq t_\epsilon$,
\[
\| \Delta_t \|_2 \leq 2\eta M^2 C_0 B^{t-1} R_0 \tilde{d}^{-1/4}
\]

and particularly we have
\[
\left\| \sqrt{Q} \Delta_t \right\|_2 \leq \| \Delta_t \|_2 \leq 2\epsilon t \eta M^2 C_0 B^{t-1} R_0 \tilde{d}^{-1/4}
\]

For $t \geq t_\epsilon$, we have the alternative update rule (52). Thus,
\[
\sqrt{Q} \Delta_{t+1} - \sqrt{Q} \Delta_t = \eta \sqrt{Q} \left[ J(\theta^{(t)})^\top J(\theta^{(0)}) - J(\theta^{(0)})^\top J(\theta^{(0)}) \right] \sqrt{Q^{(t)}_\Theta} \left[ \sqrt{Q} g(\theta^{(t)}) \right] \\
- \eta \sqrt{Q} J(\theta^{(0)})^\top J(\theta^{(0)}) \sqrt{Q^{(t)}_\Theta} \left[ \sqrt{Q} \Delta_t \right]
\]

Let $A = I - \eta \sqrt{Q} J(\theta^{(0)})^\top J(\theta^{(0)}) \sqrt{Q^{(t)}_\Theta} = I - \eta \sqrt{Q} g(\Theta^{(t)}) \sqrt{Q^{(t)}_\Theta}$. Then, we have
\[
\sqrt{Q} \Delta_{t+1} = A \sqrt{Q} \Delta_t + \eta \sqrt{Q} \left[ J(\theta^{(t)})^\top J(\theta^{(t)}) - J(\theta^{(0)})^\top J(\theta^{(0)}) \right] \sqrt{Q^{(t)}_\Theta} \left( \sqrt{Q} g(\theta^{(t)}) \right)
\]

Let $\gamma = 1 - \frac{\eta M^2}{\epsilon} < 1$. Combining with Theorem D.3 and (72), the above leads to
\[
\left\| \sqrt{Q} \Delta_{t+1} \right\|_2 \leq \| A \|_2 \left\| \sqrt{Q} \Delta_t \right\|_2 + \eta \left\| \sqrt{Q} \left[ J(\theta^{(t)})^\top J(\theta^{(t)}) - J(\theta^{(0)})^\top J(\theta^{(0)}) \right] \right\|_2 \sqrt{Q^{(t)}_\Theta} \left\| \sqrt{Q} g(\theta^{(t)}) \right\|_2 \\
\leq \gamma \left\| \sqrt{Q} \Delta_t \right\|_2 + \eta \left\| J(\theta^{(t)})^\top J(\theta^{(t)}) - J(\theta^{(0)})^\top J(\theta^{(0)}) \right\|_F \sqrt{1 + 3\epsilon \gamma^{t-t_\epsilon}} B^{t_\epsilon} R_0 \\
\leq \gamma \left\| \sqrt{Q} \Delta_t \right\|_2 + 2\eta M^2 C_0 \sqrt{1 + 3\epsilon \gamma^{t-t_\epsilon}} B^{t_\epsilon} R_0 \tilde{d}^{-1/4}
\]

This implies that
\[
\gamma^{-(t+1)} \left\| \sqrt{Q} \Delta_{t+1} \right\|_2 \leq \gamma^{- t} \left\| \sqrt{Q} \Delta_t \right\|_2 + 2\eta M^2 C_0 \sqrt{1 + 3\epsilon \gamma^{- t-t_\epsilon}} B^{t_\epsilon} R_0 \tilde{d}^{-1/4}
\]

Combining with (80), it implies that for all $t \geq t_\epsilon$,
\[
\left\| \sqrt{Q} \Delta_t \right\|_2 \leq 2\gamma^{t-t_\epsilon} \eta M^2 C_0 B^{t_\epsilon} R_0 \left[ t_\epsilon B^{-1} + \sqrt{1 + 3\epsilon \gamma^{- t-t_\epsilon}} (t - t_\epsilon) \right] \tilde{d}^{-1/4}
\]

Next, we consider an arbitrary test point $x$ such that $\| x \|_2 \leq 1$. Denote $\delta_t = f_{\text{lin}}^{(t)}(x) - f^{(t)}(x)$. Then we have
\[
\left\{ \begin{array}{l}
  f_{\text{lin}}^{(t+1)}(x) - f_{\text{lin}}^{(t)}(x) = -\eta \nabla_x f(x; \theta^{(0)})^\top J(\theta^{(0)}) Q^{(t)} g_{\text{lin}}(\theta^{(t)}) \\
  f^{(t+1)}(x) - f^{(t)}(x) = -\eta \nabla_x f(x; \theta^{(t)})^\top J(\theta^{(t)}) Q^{(t)} g(\theta^{(t)})
\end{array} \right.
\]

Understanding Why Generalized Reweighting Does Not Improve Over ERM
which yields

\[
\delta_{t+1} - \delta_t = \eta \left[ \nabla_\theta f(x; \tilde{\theta}^{(s)})^T J(\theta^{(s)}) - \nabla_\theta f(x; \theta^{(0)})^T J(\theta^{(0)}) \right] Q^{(s)} g(\theta^{(s)}) \\
- \eta \nabla_\theta f(x; \theta^{(0)})^T J(\theta^{(0)}) Q^{(s)} \Delta_t
\] (87)

For \( t \leq t_\epsilon \), we have

\[
\|\delta_t\|_2 \leq \eta \sum_{s=0}^{t-1} \left\| \left[ \nabla_\theta f(x; \tilde{\theta}^{(s)})^T J(\theta^{(s)}) - \nabla_\theta f(x; \theta^{(0)})^T J(\theta^{(0)}) \right] Q^{(s)} \right\|_2 \| g(\theta^{(s)}) \|_2 \\
+ \eta \sum_{s=0}^{t-1} \left\| \nabla_\theta f(x; \theta^{(0)})^T J(\theta^{(0)}) Q^{(s)} \right\|_2 \| \Delta_s \|_2
\leq \eta \sum_{s=0}^{t-1} \left\| \nabla_\theta f(x; \tilde{\theta}^{(s)})^T J(\theta^{(s)}) - \nabla_\theta f(x; \theta^{(0)})^T J(\theta^{(0)}) \right\|_F \| g(\theta^{(s)}) \|_2 \\
+ \eta \sum_{s=0}^{t-1} \left\| \nabla_\theta f(x; \theta^{(0)}) \right\|_2 \| J(\theta^{(0)}) \|_F \| \Delta_s \|_2
\leq 2\eta M^2 C_0 \tilde{d}^{-1/4} \sum_{s=0}^{t-1} B^s R_0 + \eta M^2 \sum_{s=0}^{t-1} (2\eta M^2 C_0 B^{s-1} R_0 \tilde{d}^{-1/4})
\] (88)

So we can see that there exists a constant \( C_1 \) such that \( \|\delta_t\|_2 \leq C_1 \tilde{d}^{-1/4} \). Then, for \( t > t_\epsilon \), we have

\[
\|\delta_t\|_2 - \|\delta_{t_\epsilon}\|_2 \leq \eta \sum_{s=t_\epsilon}^{t-1} \left\| \left[ \nabla_\theta f(x; \tilde{\theta}^{(s)})^T J(\theta^{(s)}) - \nabla_\theta f(x; \theta^{(0)})^T J(\theta^{(0)}) \right] Q^{(s)} \right\|_2 \| \sqrt{Q} g(\theta^{(s)}) \|_2 \\
+ \eta \sum_{s=t_\epsilon}^{t-1} \left\| \nabla_\theta f(x; \theta^{(0)})^T J(\theta^{(0)}) \sqrt{Q}^{(s)} \right\|_2 \| \sqrt{Q} \Delta_s \|_2
\leq 2\eta M^2 C_0 \tilde{d}^{-1/4} \sqrt{t + 3\epsilon} \sum_{s=t_\epsilon}^{t-1} \gamma^{s-t_\epsilon} B^s R_0
\]

\[
+ \eta M^2 \sqrt{t + 3\epsilon} \sum_{s=t_\epsilon}^{t-1} \left( 2\gamma^{s-t_\epsilon} \eta M^2 C_0 B^{s-1} R_0 \left[ t_\epsilon B^{-1} + \sqrt{t + 3\epsilon} \gamma^{-(s-t_\epsilon)} \right] \tilde{d}^{-1/4} \right)
\] (89)

Note that \( \sum_{t=0}^{\infty} t \gamma^t \) is finite as long as \( \gamma \in (0, 1) \). Therefore, there is a constant \( C \) such that for any \( t \), \( \|\delta_t\|_2 \leq C \tilde{d}^{-1/4} \) with probability at least \((1 - \delta)\) for any \( \tilde{d} \geq \tilde{D} \).

D.3.3. PROOF OF LEMMA D.4

We will use the following theorem regarding the eigenvalues of random Gaussian matrices:

**Theorem D.5** (Corollary 5.35 in (Vershynin, 2010)). If \( A \in \mathbb{R}^{p \times q} \) is a random matrix whose entries are independent standard normal random variables, then for every \( t \geq 0 \), with probability at least \( 1 - 2 \exp(-t^2/2) \),

\[
\sqrt{p} - \sqrt{q} - t \leq \lambda^{\min}(A) \leq \lambda^{\max}(A) \leq \sqrt{p} + \sqrt{q} + t
\] (90)

By this theorem, and also note that \( W^L \) is a vector, we can see that for any \( \delta \), there exist \( \tilde{D} > 0 \) and \( M_1 > 0 \) such that if \( \tilde{d} \geq \tilde{D} \), then with probability at least \((1 - \delta)\), for all \( \theta \in B(\theta^{(0)}, C_0) \), we have

\[
\|W^l\|_2 \leq 3\sqrt{\tilde{d}} \quad (\forall 0 \leq l \leq L - 1) \quad \text{and} \quad \|W^L\|_2 \leq C_0 \leq 3\sqrt{d}
\] (91)

as well as

\[
\|\beta b^l\|_2 \leq M_1 \sqrt{d} \quad (\forall l = 0, \cdots, L)
\] (92)
Now we assume that (91) and (92) are true. Then, for any $\mathbf{x}$ such that $\|\mathbf{x}\|_2 \leq 1$,

$$
\|h^i\|_2 = \left\| \frac{1}{\sqrt{d_0}} W_0^i \mathbf{x} + \beta^i \right\|_2 \leq \frac{1}{\sqrt{d_0}} \|W_0^i\|_2 \|\mathbf{x}\|_2 + \|\beta^i\|_2 \leq \left( \frac{3}{\sqrt{d_0}} + 1 \right) \sqrt{d} 
$$

$$
\|h^{i+1}\|_2 = \left\| \frac{1}{\sqrt{d}} W^i \mathbf{x}^i + \beta^i \right\|_2 \leq \frac{1}{\sqrt{d}} \|W^i\|_2 \|\mathbf{x}^i\|_2 + \|\beta^i\|_2 \quad (\forall i \geq 1)
$$

where $L_0$ is the Lipschitz constant of $\sigma$ and $\sigma(0^i) = (\sigma(0), \ldots, \sigma(0)) \in \mathbb{R}^{d_i}$. By induction, there exists an $M_2 > 0$ such that $\|\mathbf{x}^i\|_2 \leq M_2 \sqrt{d}$ and $\|h^i\|_2 \leq M_2 \sqrt{d}$ for all $i = 1, \ldots, L$. 

Denote $\mathbf{\alpha}^i = \nabla_{h^i} f(x) = \nabla_{h^i} \mathbf{h}^{i+1}$. For all $l = 1, \ldots, L$, we have $\mathbf{\alpha}^i = \text{diag}(\sigma(h^i))^\top \mathbf{\alpha}^{i+1} \mathbf{x}^i$ where $\sigma(x) \leq L_0$ for all $x \in \mathbb{R}$ since $\sigma$ is $L_0$-Lipschitz, $\mathbf{\alpha}^{i+1} = 1$ and $\|\mathbf{\alpha}^i\|_2 = \left\| \text{diag}(\sigma(h^i))^\top \mathbf{\alpha}^{i+1} \right\|_2 \leq \frac{3}{\sqrt{d}} L_0$. Then, we can easily prove by induction that there exists an $M_3 > 1$ such that $\|\mathbf{\alpha}^i\|_2 \leq M_3 \sqrt{d}$ for all $i = 1, \ldots, L$ (note that this is not true for $L + 1$ because $\mathbf{\alpha}^{L+1} = \mathbf{1}$).

For $l = 0$, $\nabla W_0 f(x) = \frac{1}{\sqrt{d_0}} \mathbf{x}^0 \mathbf{\alpha}^1$, so $\|\nabla W_0 f(x)\|_2 \leq \frac{1}{\sqrt{d_0}} \|\mathbf{x}^0\|_2 \|\mathbf{\alpha}^1\|_2 \leq \frac{1}{\sqrt{d_0}} M_3 \sqrt{d}$. And for any $l = 1, \ldots, L$, $\nabla W_l f(x) = \frac{1}{\sqrt{d}} \mathbf{x}^{l+1} \mathbf{\alpha}^{l+1}$, so $\|\nabla W_l f(x)\|_2 \leq \frac{1}{\sqrt{d}} \|\mathbf{x}^{l+1}\|_2 \|\mathbf{\alpha}^{l+1}\|_2 \leq M_2 M_3$. (Note that if $M_3 > 1$, then $\|\mathbf{\alpha}^{L+1}\|_2 \leq M_3$; and since $\sqrt{d} \geq 1$, there is $\|\mathbf{\alpha}^i\|_2 \leq M_3$ for $l \leq L$.) Moreover, for $l = 0, \ldots, L$, $\nabla \theta f(x) = \beta \mathbf{\alpha}^{l+1}$, so $\|\nabla \theta f(x)\|_2 \leq \beta M_3$. Thus, if (91) and (92) are true, then there exists an $M_4 > 0$, such that $\|\nabla \theta f(x)\|_2 \leq M_4 \sqrt{n}$. And since $\|\mathbf{x}^i\|_2 \leq 1$ for all $i$, so $J(\theta) \|F\|_F \leq M_4$.

Next, we consider the difference in $\nabla \theta f(x)$ between $\theta$ and $\tilde{\theta}$. Let $\hat{f}, \hat{W}, \hat{b}, \hat{x}, \hat{h}, \hat{\alpha}$ be the function and the values corresponding to $\tilde{\theta}$. There is

$$
\|h^1 - \hat{h}^1\|_2 = \left\| \frac{1}{\sqrt{d_0}} (W_0^1 - \hat{W}_0) \mathbf{x} + \beta^0 (\hat{b}^0 - \hat{\beta}^0) \right\|_2 
$$

$$
\leq \frac{1}{\sqrt{d_0}} \|W_0^1 - \hat{W}_0\|_2 \|\mathbf{x}\|_2 + \beta^0 \|\hat{b}^0 - \hat{\beta}^0\|_2 \leq \left( \frac{1}{\sqrt{d_0}} + \beta \right) \|\theta - \tilde{\theta}\|_2 
$$

$$
\|h^{i+1} - \hat{h}^{i+1}\|_2 = \left\| \frac{1}{\sqrt{d}} W^i (\mathbf{x}^i - \hat{\mathbf{x}}^i) + \frac{1}{\sqrt{d}} (W^i - \hat{W}^i) \mathbf{x}^i + \beta^i (\hat{b}^i - \hat{\beta}^i) \right\|_2 
$$

$$
\leq \frac{1}{\sqrt{d}} \|W^i\|_2 \|\mathbf{x}^i - \hat{\mathbf{x}}^i\|_2 + \frac{1}{\sqrt{d}} \|W^i - \hat{W}^i\|_2 \|\mathbf{x}^i\|_2 + \beta \|\hat{b}^i - \hat{\beta}^i\|_2 
$$

$$
\leq 3 \|\mathbf{x}^i - \hat{\mathbf{x}}^i\|_2 + (M_2 + \beta) \|\theta - \tilde{\theta}\|_2 \quad (\forall i \geq 1)
$$

$$
\|\mathbf{x}^i - \hat{\mathbf{x}}^i\|_2 = \left\| \sigma(h^i) - \sigma(\hat{h}^i) \right\|_2 \leq L_0 \|h^i - \hat{h}^i\|_2 \quad (\forall i \geq 1)
$$

By induction, there exists an $M_5 > 0$ such that $\|\mathbf{x}^i - \hat{\mathbf{x}}^i\|_2 \leq M_5 \|\theta - \tilde{\theta}\|_2$ for all $i$. 

Understanding Why Generalized Reweighting Does Not Improve Over ERM
Understanding Why Generalized Reweighting Does Not Improve Over ERM

For $\alpha^l$, we have $\alpha^{L+1} = \hat{\alpha}^{L+1} = 1$, and for all $l \geq 1,$

$$
\|\alpha^l - \hat{\alpha}^l\|_2 = \left\| \text{diag}(\hat{\alpha}^l) \frac{W_l^* \alpha^{l+1} - \text{diag}(\hat{\alpha}^l) \hat{W}_l^* \hat{\alpha}^{l+1}}{\sqrt{d}} \right\|_2 \\
\leq \left\| \text{diag}(\hat{\alpha}^l) \frac{W_l^* (\alpha^{l+1} - \hat{\alpha}^{l+1})}{\sqrt{d}} \right\|_2 + \left\| \text{diag}(\hat{\alpha}^l) \frac{(W_l^* - \hat{W}_l^*)^T \hat{\alpha}^{l+1}}{\sqrt{d}} \right\|_2 \\
+ \left\| \text{diag}(\hat{\alpha}^l) \frac{(\hat{\alpha}^l - \hat{\alpha}^l) \hat{W}_l^*}{\sqrt{d}} \hat{\alpha}^{l+1} \right\|_2 \\
\leq 3L_0 \|\alpha^{l+1} - \hat{\alpha}^{l+1}\|_2 + \left( M_3L_0 \tilde{d}^{-1/2} + 3M_3M_5L_1 \tilde{d}^{-1/4} \right) \|\theta - \hat{\theta}\|_2 
$$

(95)

where $L_1$ is the Lipschitz constant of $\hat{\sigma}$. Particularly, for $l = L$, though $\hat{\alpha}^{L+1} = 1$, since $\|\hat{W}_L^*\|_2 \leq 3\tilde{d}^{1/4}$, (95) is still true.

By induction, there exists an $M_0 > 0$ such that $\|\alpha^l - \hat{\alpha}^l\|_2 \leq \frac{M_0}{\sqrt{d}} \|\theta - \hat{\theta}\|_2$ for all $l \geq 1$ (note that this is also true for $l = L + 1$).

Thus, if (91) and (92) are true, then for all $\theta, \hat{\theta} \in B(\theta^{(0)}, C_0)$, any $x$ such that $\|x\|_2 \leq 1$, we have

$$
\left\| \nabla_{W^0} f(x) - \nabla_{\tilde{W}^0} \tilde{f}(x) \right\|_2 = \frac{1}{\sqrt{d_0}} \left\| x^\top \alpha^{1T} - x^\top \hat{\alpha}^{1T} \right\|_2 \\
\leq \frac{1}{\sqrt{d_0}} \|\alpha^1 - \hat{\alpha}^1\|_2 \\
\leq \frac{1}{\sqrt{d_0}} \frac{M_6}{\sqrt{d}} \|\theta - \hat{\theta}\|_2 
$$

(96)

and for $l = 1, \cdots, L$, we have

$$
\left\| \nabla_{W^l} f(x) - \nabla_{\tilde{W}^l} \tilde{f}(x) \right\|_2 = \frac{1}{\sqrt{d}} \left\| x^\top \alpha^{l+1T} - x^\top \hat{\alpha}^{l+1T} \right\|_2 \\
\leq \frac{1}{\sqrt{d}} \left( \left\| x^\top \right\|_2 \left\| \alpha^{l+1} - \hat{\alpha}^{l+1}\right\|_2 + \left\| x^\top - \hat{x}^\top \right\|_2 \left\| \hat{\alpha}^{l+1}\right\|_2 \right) \\
\leq \left( \frac{M_3M_6}{\sqrt{d}} + \frac{M_5M_3}{\sqrt{d}} \right) \|\theta - \hat{\theta}\|_2 
$$

(97)

Moreover, for any $l \in \{0, \cdots, L\}$, there is

$$
\left\| \nabla_{\theta^l} f(x) - \nabla_{\hat{\theta}^l} \hat{f}(x) \right\|_2 = \beta \left\| \alpha^{l+1} - \hat{\alpha}^{l+1}\right\|_2 \leq \frac{\beta M_6}{\sqrt{d}} \|\theta - \hat{\theta}\|_2 
$$

(98)

Overall, we can see that there exists a constant $M_7 > 0$ such that $\left\| \nabla_{\theta} f(x) - \nabla_{\hat{\theta}} \hat{f}(x) \right\|_2 \leq \frac{M_7}{\sqrt{d}} \|\theta - \hat{\theta}\|_2$, so that

$$
\| f(\theta) - f(\hat{\theta}) \|_F \leq \frac{M_7}{\sqrt{d}} \|\theta - \hat{\theta}\|_2. 
$$

D.3.4. Proof of Theorem 4.4

First of all, for a linearized neural network (13), if we view $\{\nabla_{\theta} f^{(0)}(x_i)\}_{i=1}^{n}$ as the inputs and $\{y_i - f^{(0)}(x_i) + (\theta^{(0)}(x_i) \nabla_{\theta} f^{(0)}(x_i))\}_{i=1}^{n}$ as the targets, then the model becomes a linear model. So by Theorem 4.2 we have the following corollary:

**Corollary D.6.** If $\nabla_{\theta} f^{(0)}(x_1), \cdots, \nabla_{\theta} f^{(0)}(x_n)$ are linearly independent, then there exists $\eta_0 > 0$ such that for any GRW satisfying Assumption 1, and any $\eta \leq \eta_0$, $\theta^{(t)}$ converges to the same interpolator $\theta^*$ that does not depend on $q_t$. 


Let $\eta_1 = \min \{ \eta_0, \eta^* \}$, where $\eta_0$ is defined in Corollary D.6 and $\eta^*$ is defined in Lemma 4.5. Let $f^{(t)}_{\text{lin}}(x)$ and $f^{(t)}_{\text{linERM}}(x)$ be the linearized neural networks of $f^{(t)}(x)$ and $f^{(t)}_{\text{ERM}}(x)$, respectively. By Lemma 4.5, for any $\delta > 0$, there exists $D > 0$ and a constant $C$ such that

$$
\begin{align*}
&\sup_{t \geq 0} \left| f^{(t)}_{\text{lin}}(x) - f^{(t)}(x) \right| \leq C d^{-1/4} \\
&\sup_{t \geq 0} \left| f^{(t)}_{\text{linERM}}(x) - f^{(t)}_{\text{ERM}}(x) \right| \leq C d^{-1/4}
\end{align*}
$$

(99)

By Corollary D.6, we have

$$
\lim_{t \to \infty} \left| f^{(t)}_{\text{lin}}(x) - f^{(t)}_{\text{linERM}}(x) \right| = 0
$$

(100)

Summing the above yields

$$
\limsup_{t \to \infty} \left| f^{(t)}(x) - f^{(t)}_{\text{ERM}}(x) \right| \leq 2C d^{-1/4}
$$

(101)

which is the result we want.

\[ \square \]

D.4. Proofs for Subsection 4.3

D.4.1. A NEW APPROXIMATION THEOREM

**Lemma D.7** (Approximation Theorem for Regularized GRW). For a wide fully-connected neural network $f$, denote $J(\theta) = \nabla_{\theta} f(X; \theta) \in \mathbb{R}^{p \times n}$ and $g(\theta) = \nabla_{\theta} \ell(f(X; \theta), Y) \in \mathbb{R}^n$. Given that the loss function $\ell$ satisfies: $\nabla_a g(\theta) = J(\theta) U(\theta)$ for any $\theta$, and $U(\theta)$ is a positive semi-definite diagonal matrix whose elements are uniformly bounded, we have: for any $\text{GRW}$ that minimizes the regularized weighted empirical risk (15) with a sufficiently small learning rate $\eta$, there is: for a sufficiently large $d$, with high probability over random initialization, on any test point $x$ such that $\|x\|_2 \leq 1$,

$$
\sup_{t \geq 0} \left| f^{(t)}_{\text{linrad}}(x) - f^{(t)}_{\text{reg}}(x) \right| \leq C d^{-1/4}
$$

(102)

where both $f^{(t)}_{\text{linrad}}$ and $f^{(t)}_{\text{reg}}$ are trained by the same regularized GRW and start from the same initial point.

First of all, with some simple linear algebra analysis, we can prove the following proposition:

**Proposition D.8.** For any positive definite symmetric matrix $H \in \mathbb{R}^{n \times n}$, denote its largest and smallest eigenvalues by $\lambda^\max$ and $\lambda^\min$. Then, for any positive semi-definite diagonal matrix $Q = \text{diag}(q_1, \cdots, q_n)$, $HQ$ has $n$ eigenvalues that all lie in $[\min(q_1 \cdots q_n, \lambda^\min), \min(q_1 \cdots q_n, \lambda^\max)]$.

**Proof.** $H$ is a positive definite symmetric matrix, so there exists $A \in \mathbb{R}^{n \times n}$ such that $H = A^T A$, and $A$ is full-rank. First, any eigenvalue of $AQ A^T$ is also an eigenvalue of $A^T A Q$, because for any eigenvalue $\lambda$ of $AQ A^T$ we have some $v \neq 0$ such that $AQ A^T v = \lambda v$. Multiplying both sides by $A^T$ on the left yields $A^T AQ(A^T v) = \lambda(A^T v)$, which implies that $\lambda$ is also an eigenvalue of $A^T A Q$ because $A^T v 
eq 0$ as $\lambda v \neq 0$.

Second, by condition we know that the eigenvalues of $A^T A$ are all in $[\lambda^\min, \lambda^\max]$ where $\lambda^\min > 0$, which implies for any unit vector $v$, $v^T A^T A v \in [\lambda^\min, \lambda^\max]$, which is equivalent to $\| A v \|_2 \in [\sqrt{\lambda^\min}, \sqrt{\lambda^\max}]$. Thus, we have $v^T A^T Q A v \in [\lambda^\min \min(q_1 \cdots q_n, \lambda^\max)]$, which implies that the eigenvalues of $A^T Q A$ are all in $[\lambda^\min \min(q_1 \cdots q_n, \lambda^\max)]$.

Thus, the eigenvalues of $H Q = A^T A Q$ are all in $[\lambda^\min \min(q_1 \cdots q_n, \lambda^\max)]$.

**Proof of Lemma D.7** By the condition $\ell$ satisfies, without loss of generality, assume that the elements of $U(\theta)$ are in $[0, 1]$ for all $\theta$. Then, let $\eta \leq (\mu + C \lambda^\min + C \lambda^\max)^{-1}$. (If the elements of $U(\theta)$ are bounded by $[0, C]$, then we can let $\eta \leq (\mu + C \lambda^\min + C \lambda^\max)^{-1}$ and prove the result in the same way.)

With $L_2$ penalty, the update rule of the GRW for the neural network is:

$$
\theta^{(t+1)} = \theta^{(t)} - \eta J(\theta^{(t)}) Q^{(t)} g(\theta^{(t)}) - \eta \mu (\theta^{(t)} - \theta^{(0)})
$$

(103)

And the update rule for the linearized neural network is:

$$
\theta_{\text{lin}}^{(t+1)} = \theta_{\text{lin}}^{(t)} - \eta J(\theta^{(0)}) Q^{(t)} g(\theta_{\text{lin}}^{(t)}) - \eta \mu (\theta_{\text{lin}}^{(t)} - \theta^{(0)})
$$

(104)
By Proposition D.2, $f(x; \theta)$ converges in probability to a zero-mean Gaussian process. Thus, for any $\delta > 0$, there exists a constant $R_0 > 0$ such that with probability at least $(1 - \delta/3)$, $\|g(\theta(t))\|_2 < R_0$. Let $M$ be as defined in Lemma D.4. Denote $A = \eta M R_0$, and let $C_0 = \frac{4A}{\eta^2}$ in Lemma D.4. By Lemma D.4, there exists $D_1$ such that for all $d \geq D_1$, with probability at least $(1 - \delta/3)$, (57) is true.

Similar to the proof of Proposition D.8, we can show that for arbitrary $\tilde{\theta}$, all non-zero eigenvalues of $J(\theta(0))Q^{(t)}U(\tilde{\theta})J(\theta(0))^T$ are eigenvalues of $J(\theta(t))J(\theta(0))Q^{(t)}U(\tilde{\theta})$. This is because for any $\lambda \neq 0$, if $\lambda v = \lambda J(\theta(t))J(\theta(0))Q^{(t)}U(\tilde{\theta})v$, then $\lambda v = \lambda J(\theta(t))J(\theta(0))Q^{(t)}U(\tilde{\theta})v = \lambda J(\theta(t))J(\theta(0))Q^{(t)}U(\tilde{\theta})v = \lambda J(\theta(t))J(\theta(0))Q^{(t)}U(\tilde{\theta})v = \lambda J(\theta(t))J(\theta(0))Q^{(t)}U(\tilde{\theta})v$ since $\lambda v \neq 0$, so $\lambda$ is also an eigenvalue of $J(\theta(t))J(\theta(0))Q^{(t)}U(\tilde{\theta})$. On the other hand, by Proposition 4.3, $J(\theta(t))^TJ(\theta(t))Q^{(t)}U(\tilde{\theta})$ converges in probability to $\Theta Q^{(t)}U(\tilde{\theta})$ whose eigenvalues are all in $[0,\lambda_{\text{max}}]$ by Proposition D.8.

So there exists $D_2$ such that for all $d \geq D_2$, with probability at least $(1 - \delta/3)$, the eigenvalues of $J(\theta(t))Q^{(t)}U(\tilde{\theta})J(\theta(0))^T$ are all in $[0,\lambda_{\text{max}} + \lambda_{\text{min}}]$ for all $t$.

By union bound, with probability at least $(1 - \delta)$, all three above are true, which we will assume in the rest of this proof.

First, we need to prove that there exists $D_3$ such that for all $d \geq D_3$, $\sup_{t \geq 0} \|\tilde{\theta}(t) - \theta(0)\|_2$ is bounded with high probability. Denote $a_t = \tilde{\theta}(t) - \theta(t)$.

By (103) we have

$$a_{t+1} = (1 - \eta \mu) a_t - \eta J(\theta(t)) J(\theta(0)) g(\theta(t)) - \eta J(\theta(t)) Q^{(t)} [g(\theta(t)) - g(\theta(0))] - \eta J(\theta(t)) Q^{(t)} g(\theta(0))$$

where $\tilde{\theta}(t)$ is some linear interpolation between $\theta(t)$ and $\theta(0)$. Our choice of $\eta$ ensures that $\eta \mu < 1$.

Now we prove by induction that $\|a_t\|_2 < C_0$. It is true for $t = 0$, so we need to prove that if $\|a_t\|_2 < C_0$, then $\|a_{t+1}\|_2 < C_0$.

For the first term on the right-hand side of (106), we have

$$\|J(\theta(t))Q^{(t)}U(\tilde{\theta}(t))J(\theta(0))^T\|_2 \leq \|J(\theta(0))Q^{(t)}U(\tilde{\theta}(t))J(\theta(0))^T\|_2 + \eta \|J(\theta(t)) - J(\theta(0))\|_F \|g(\theta(t))\|_2$$

Since $\eta/(1 - \eta \mu) \leq (\lambda_{\text{min}} + \lambda_{\text{max}})^{-1}$ by our choice of $\eta$, we have

$$\|I - \frac{\eta}{1 - \eta \mu} J(\theta(t))Q^{(t)}U(\tilde{\theta}(t))J(\theta(0))^T\|_2 \leq 1$$

On the other hand, we can use (57) since $\|a_t\|_2 < C_0$, so $\|J(\theta(t))Q^{(t)}U(\tilde{\theta}(t))J(\theta(0))^T\|_2 \leq M^2 \sqrt{d} C_0$. Therefore, there exists $D_3$ such that for all $d \geq D_3$, $\|a_{t+1}\|_2 \leq 1 - \eta \mu$.

For the second term, we have

$$\|g(\theta(t))\|_2 \leq \|g(\theta(t)) - g(\theta(0))\|_2 + \|g(\theta(0))\|_2$$

Note that Lemma D.4 only depends on the network structure and does not depend on the update rule, so we can use this lemma here.
And for the third term, we have
\[ \eta \left\| J(\theta^{(0)}) \right\|_F \left\| g(\theta^{(0)}) \right\|_2 \leq \eta MR_0 = A \] (111)

Thus, we have
\[ \|a_{t+1}\|_2 \leq \left( 1 - \frac{\eta \mu}{2} \right) \|a_t\|_2 + \frac{\eta M(MC_0 + R_0)}{\sqrt{d}} + A \] (112)

So there exists \( D_4 \) such that for all \( \tilde{d} \geq D_4 \), \( \|a_{t+1}\|_2 \leq (1 - \frac{\eta \mu}{2}) \|a_t\|_2 + 2A \). This shows that if \( \|a_t\|_2 < C_0 \) is true, then \( \|a_{t+1}\|_2 < C_0 \) will also be true.

In conclusion, for all \( \tilde{d} \geq D_0 = \max\{D_1, D_2, D_3, D_4\} \), \( \|\theta^{(t)} - \theta^{(0)}\|_2 < C_0 \) is true for all \( t \). This also implies that for \( C_1 = MC_0 + R_0 \), we have \( \|g(\theta^{(t)})\|_2 \leq C_1 \) for all \( t \) by (110). Similarly, we can prove that \( \|\theta_{lin}^{(t)} - \theta^{(0)}\|_2 < C_0 \) for all \( t \).

Second, let \( \Delta_t = \theta_{lin}^{(t)} - \theta^{(t)} \). Then we have
\[ \Delta_{t+1} - \Delta_t = \eta (J(\theta^{(t)}) Q^{(t)} g(\theta^{(t)}) - J(\theta^{(0)}) Q^{(t)} g(\theta_{lin}^{(t)}) - \mu \Delta_t) \] (113)

which implies
\[ \Delta_{t+1} = \left[ (1 - \eta \mu) I - \eta J(\theta^{(0)}) Q^{(t)} U(\hat{\theta}(t)) J(\hat{\theta}(t))^\top \right] \Delta_t + \eta (J(\theta^{(t)}) - J(\theta^{(0)})) Q^{(t)} g(\theta^{(t)}) \] (114)

where \( \hat{\theta}(t) \) is some linear interpolation between \( \theta^{(t)} \) and \( \theta_{lin}^{(t)} \). By (109), with probability at least \( (1 - \delta) \) for all \( \tilde{d} \geq D_0 \), we have
\[ \|\Delta_{t+1}\|_2 \leq \left\| (1 - \eta \mu) I - \eta J(\theta^{(0)}) Q^{(t)} U(\hat{\theta}(t)) J(\hat{\theta}(t))^\top \right\|_2 \|\Delta_t\|_2 + \eta \left\| J(\theta^{(t)}) - J(\theta^{(0)}) \right\|_F \left\| g(\theta^{(t)}) \right\|_2 \] (115)

Again, as \( \Delta_0 = 0 \), we can prove by induction that for all \( t \),
\[ \|\Delta_t\|_2 \leq \frac{2MC_0 C_1}{\mu} \tilde{d}^{-1/4} \] (116)

For any test point \( x \) such that \( \|x\|_2 \leq 1 \), we have
\[ \left| f_{reg}^{(t)}(x) - f_{linreg}^{(t)}(x) \right| = \left| f(x; \theta^{(t)}) - f_{lin}(x; \theta_{lin}^{(t)}) \right| \leq \left| f(x; \theta^{(t)}) - f_{lin}(x; \theta^{(t)}) \right| + \left| f_{lin}(x; \theta^{(t)}) - f_{lin}(x; \theta_{lin}^{(t)}) \right| \] (117)

For the first term, note that
\[ \begin{cases} f(x; \theta^{(t)}) - f(x; \theta^{(0)}) = \nabla_{\theta} f(x; \hat{\theta}(t))(\theta^{(t)} - \theta^{(0)}) \\ f_{lin}(x; \theta^{(t)}) - f_{lin}(x; \theta^{(0)}) = \nabla_{\theta} f(x; \theta^{(0)})(\theta^{(t)} - \theta^{(0)}) \end{cases} \] (118)

where \( \hat{\theta}(t) \) is some linear interpolation between \( \theta^{(t)} \) and \( \theta^{(0)} \). Since \( f(x; \theta^{(0)}) = f_{lin}(x; \theta^{(0)}) \),
\[ \left| f(x; \theta^{(t)}) - f_{lin}(x; \theta^{(t)}) \right| \leq \left\| \nabla_{\theta} f(x; \hat{\theta}(t)) - \nabla_{\theta} f(x; \theta^{(0)}) \right\|_2 \left\| \theta^{(t)} - \theta^{(0)} \right\|_2 \leq \frac{M}{\sqrt{d}} C_0^2 \] (119)

Thus, we have shown that for all \( \tilde{d} \geq D_0 \), with probability at least \( (1 - \delta) \) for all \( t \) and all \( x \),
\[ \left| f_{reg}^{(t)}(x) - f_{linreg}^{(t)}(x) \right| \leq \left( MC_0^2 + \frac{2M^2C_0 C_1}{\mu} \right) \tilde{d}^{-1/4} = O(\tilde{d}^{-1/4}) \] (120)

which is the result we need.
D.4.2. Result for Linearized Neural Networks

Lemma D.9. Suppose there exists $M_0 > 0$ such that $\|\nabla \hat{f}^{(0)}(x)\|_2 \leq M_0$ for all test point $x$. If the gradients $\nabla \hat{f}^{(0)}(x_1), \ldots, \nabla \hat{f}^{(0)}(x_n)$ are linearly independent, and the empirical training risk of $f^{(t)}_{\text{linereg}}$ satisfies

$$\limsup_{t \to \infty} \hat{\mathcal{R}}(f^{(t)}_{\text{linereg}}) < \epsilon,$$

for some $\epsilon > 0$, then for $x$ such that $\|x\|_2 \leq 1$ we have

$$\limsup_{t \to \infty} |f^{(t)}_{\text{linereg}}(x) - f^{(t)}_{\text{linERM}}(x)| = O(\sqrt{\epsilon}).$$

First, we can see that under the new weight update rule, $\theta(t) - \theta(0) \in \text{span}(\nabla \hat{f}^{(0)}(x_1), \ldots, \nabla \hat{f}^{(0)}(x_n))$ is still true for all $t$. Let $\theta^\star$ be the interpolator in $\text{span}(\nabla \hat{f}^{(0)}(x_1), \ldots, \nabla \hat{f}^{(0)}(x_n))$, then the empirical risk of $\theta$ is $\frac{1}{n} \sum_{i=1}^n (\theta - \theta^\star, \nabla \hat{f}^{(0)}(x_i))^2 = \frac{1}{n} \|\nabla \hat{f}^{(0)}(X)^\top (\theta - \theta^\star)\|_2^2$. Thus, there exists $T > 0$ such that for any $t \geq T$,

$$\|\nabla \hat{f}^{(0)}(X)^\top (\theta(t) - \theta^\star)\|_2^2 \leq 2\epsilon \eta$$

Let the smallest singular value of $\frac{1}{\sqrt{n}} \nabla \hat{f}^{(0)}(X)$ be $s_{\text{min}}$, and we have $s_{\text{min}} > 0$. Note that the column space of $\nabla \hat{f}^{(0)}(X)$ is exactly $\text{span}(\nabla \hat{f}^{(0)}(x_1), \ldots, \nabla \hat{f}^{(0)}(x_n))$. Define $H \in \mathbb{R}^{p \times n}$ such that its columns form an orthonormal basis of this subspace, then there exists $G \in \mathbb{R}^{n \times n}$ such that $\nabla \hat{f}^{(0)}(X) = HG$, and the smallest singular value of $\frac{1}{\sqrt{n}} G$ is also $s_{\text{min}}$. Since $\theta(t) - \theta(0)$ is also in this subspace, there exists $v \in \mathbb{R}^n$ such that $\theta(t) - \theta^\star = Hv$. Then we have $\sqrt{2\epsilon \eta} \geq \|G^\top H^\top Hv\|_2 = \|G^\top v\|_2$. Thus, $\|v\|_2 \leq \frac{\sqrt{2\epsilon}}{s_{\text{min}}}$, which implies

$$\|\theta(t) - \theta^\star\|_2 \leq \frac{\sqrt{2\epsilon}}{s_{\text{min}}}$$

We have already proved in previous results that if we minimize the unregularized risk with ERM, then $\theta$ always converges to the interpolator $\theta^\star$. So for any $t \geq T$ and any test point $x$ such that $\|x\|_2 \leq 1$, we have

$$|f^{(t)}_{\text{linereg}}(x) - f^{(t)}_{\text{linERM}}(x)| = |(\theta(t) - \theta^\star, \nabla \hat{f}^{(0)}(x))| \leq \frac{M_0 \sqrt{2\epsilon}}{s_{\text{min}}}$$

which implies (122).

D.4.3. Proof of Theorem 4.6

Given that $\hat{\mathcal{R}}(f^{(t)}_{\text{linereg}}) < \epsilon$ for sufficiently large $t$, Lemma D.7 implies that

$$\hat{\mathcal{R}}(f^{(t)}_{\text{linereg}}) - \hat{\mathcal{R}}(f^{(t)}_{\text{reg}}) = O(\tilde{d}^{-1/4} \sqrt{\epsilon} + \tilde{d}^{-1/2})$$

So for a fixed $\epsilon$, there exists $D > 0$ such that for all $d \geq D$, for sufficiently large $t$,

$$\hat{\mathcal{R}}(f^{(t)}_{\text{reg}}) < \epsilon \Rightarrow \hat{\mathcal{R}}(f^{(t)}_{\text{linereg}}) < 2\epsilon$$

By Lemma 4.5 and Lemma D.7, we have

$$\sup_{t \geq 0} |f^{(t)}_{\text{linERM}}(x) - f^{(t)}_{\text{ERM}}(x)| = O(\tilde{d}^{-1/4})$$

Combining Lemma D.9 with (128) derives

$$\limsup_{t \to \infty} |f^{(t)}_{\text{reg}}(x) - f^{(t)}_{\text{ERM}}(x)| = O(\tilde{d}^{-1/4} + \sqrt{\epsilon})$$

Letting $\tilde{d} \to \infty$ leads to the result we need.
Remark. One might wonder whether \( \| \nabla_{\theta} f^{(0)}(\theta) \|_2 \) will diverge as \( \hat{d} \to \infty \). In fact, in Lemma D.4, we have proved that there exists a constant \( M \) such that with high probability, for any \( \hat{d} \) there is \( \| \nabla_{\theta} f^{(0)}(\theta) \|_2 \leq M \) for any \( \theta \) such that \( \| \theta \|_2 \leq 1 \). Therefore, it is fine to suppose that there exists such an \( M_0 \).

D.5. Proofs for Subsection 5.1

D.5.1 Proof of Theorem 5.1

First we need to show that \( \hat{\theta}_{\text{MM}} \) is unique. Suppose both \( \theta_1 \) and \( \theta_2 \) maximize \( \min_{i=1,\ldots,n} y_i \cdot \langle \theta, x_i \rangle \) and \( \theta_1 \neq \theta_2 \). \( \| \theta_1 \|_2 = \| \theta_2 \|_2 = 1 \). Then consider \( \theta_0 = \theta/\|\theta\|_2 \) where \( \theta = (\theta_1 + \theta_2)/2 \). Obviously, \( \|\theta\|_2 < 1 \), and for any \( i, y_i \cdot \langle \theta, x_i \rangle = (y_i \cdot \langle \theta_1, x_i \rangle + y_i \cdot \langle \theta_2, x_i \rangle)/2 \), so \( y_i \cdot \langle \theta_0, x_i \rangle > \min \{ y_i \cdot \langle \theta_1, x_i \rangle, y_i \cdot \langle \theta_2, x_i \rangle \} \), which implies that \( \min_{i=1,\ldots,n} y_i \cdot \langle \theta_0, x_i \rangle > \min \{ \min_{i=1,\ldots,n} y_i \cdot \langle \theta_1, x_i \rangle, \min_{i=1,\ldots,n} y_i \cdot \langle \theta_2, x_i \rangle \} \), contradiction!

Now we start proving the result. Without loss of generality, let \( (x_1, y_1), \ldots, (x_m, y_m) \) be the samples with the smallest margin to \( \gamma_u \), i.e.,

\[
\arg \min_{1 \leq i \leq n} y_i \cdot \langle u, x_i \rangle = \{1, \ldots, m\}
\]  

(130)

And denote \( y_1 \cdot \langle u, x_1 \rangle = \cdots = y_m \cdot \langle u, x_m \rangle = \gamma_u \). Since the training error converges to 0, \( \gamma_u > 0 \). Note that for the logistic loss, if \( y_i \cdot \langle \theta, x_i \rangle < y_j \cdot \langle \theta, x_j \rangle \), then for any \( M > 0 \), there exists an \( R_M > 0 \) such that for all \( R \geq R_M \),

\[
\frac{\nabla_{\theta} \ell((R\theta, x_i), y_i)}{\nabla_{\theta} \ell((R\theta, x_j), y_i)} > M
\]  

(131)

which can be shown with some simple calculation. And because the training error converges to 0, we must have \( \| \theta(t) \| \to \infty \). Then, by Assumption 3 this means that when \( t \) gets sufficiently large, the impact of \( (x_j, y_j) \) to \( \theta(t) \) where \( j > m \) is an infinitesimal compared to \( (x_i, y_i) \) where \( i \leq m \) (because there exists a positive constant \( \delta \) such that \( q^{(t)}_{i,j} > \delta \) for all sufficiently large \( t \) by Assumption 3). Thus, we must have \( u \in \text{span}\{x_1, \ldots, x_m\} \). And in this \( m \)-dimensional linear space, there is only one unit vector \( u \) such that \( (x_1, y_1), \ldots, (x_m, y_m) \) have the same positive margin to \( u \).

Let \( u = \alpha_1 y_1 x_1 + \cdots + \alpha_m y_m x_m \). Now we show that \( \alpha_i \geq 0 \) for all \( i = 1, \ldots, m \). This is because when \( t \) is sufficiently large such that the impact of \( (x_j, y_j) \) to \( \theta(t) \) where \( j > m \) becomes infinitesimal, we have

\[
\theta(t+1) - \theta(t) \approx \frac{q^{(t)}_i \exp(y_i \cdot \langle \theta(t), x_i \rangle)}{1 + \exp(y_i \cdot \langle \theta(t), x_i \rangle)} y_i x_i
\]  

(132)

and since \( \| \theta(t) \| \to \infty \) as \( t \to \infty \), we have

\[
\alpha_i \propto \lim_{T \to \infty} \sum_{t = T_0}^{T} \frac{q^{(t)}_i \exp(y_i \cdot \langle \theta(t), x_i \rangle)}{1 + \exp(y_i \cdot \langle \theta(t), x_i \rangle)} y_i x_i \Rightarrow \lim_{T \to \infty} \alpha_i(T)
\]  

(133)

where \( T_0 \) is sufficiently large. Here the notion \( \lim_{T \to \infty} \alpha_i(T) \) means that \( \lim_{T \to \infty} \frac{\alpha_i(T)}{\alpha_j(T)} = \frac{\alpha_i}{\alpha_j} \) for any pair of \( i, j \) and \( \alpha_j \neq 0 \). Note that each term in the sum is non-negative. This implies that all \( \alpha_1, \ldots, \alpha_m \) have the same sign (or equal to 0). On the other hand,

\[
\sum_{i=1}^{m} \alpha_i y_i = \sum_{i=1}^{m} \alpha_i y_i \cdot \langle u, x_i \rangle = \langle u, u \rangle > 0
\]  

(134)

Thus, \( \alpha_i \geq 0 \) for all \( i \) and at least one of them is positive. Now suppose \( u \neq \hat{\theta}_{\text{MM}} \), which means that \( \gamma_u \) is smaller than the margin of \( \hat{\theta}_{\text{MM}} \). Then, for all \( i = 1, \ldots, m \), there is \( y_i \cdot \langle u, x_i \rangle < y_i \cdot \langle \hat{\theta}_{\text{MM}}, x_i \rangle \). This implies that

\[
\langle u, u \rangle = \sum_{i=1}^{m} \alpha_i y_i \cdot \langle u, x_i \rangle < \sum_{i=1}^{m} \alpha_i y_i \cdot \langle \hat{\theta}_{\text{MM}}, x_i \rangle = \langle \hat{\theta}_{\text{MM}}, u \rangle
\]  

(135)

which is a contradiction. Thus, we must have \( u = \hat{\theta}_{\text{MM}} \).
D.5.2. PROOF OF THEOREM 5.2

Denote the largest and smallest eigenvalues of $X^\top X$ by $\lambda_{\text{max}}$ and $\lambda_{\text{min}}$, and by condition we have $\lambda_{\text{min}} > 0$. Let $\epsilon = \min\{q_i^2, (q_i^* \lambda_{\text{min}})^2\}$. Then similar to the proof in Appendix D.2.2, there exists $t_* \epsilon$ such that for all $t \geq t_\epsilon$ and all $i$, $q_i(t) \epsilon (q_i - \epsilon, q_i + \epsilon)$. Denote $Q = \text{diag}(q_1, \ldots, q_n)$, then for all $t \geq t_\epsilon$, $Q(t) = Q(t) = \sqrt{Q(t)}$, where we use the subscript $\epsilon$ to indicate that $\|Q^\top - Q\|_2 < \epsilon$.

First, we prove that $F(\theta)$ is $L$-smooth as long as $\|x_i\|_2 \leq 1$ for all $i$. The gradient of $F$ is

$$\nabla F(\theta) = \sum_{i=1}^{n} q_i \nabla \ell(\langle \theta, x_i \rangle, y_i) x_i$$

(136)

Since $\ell(\hat{y}, y)$ is $L$-smooth in $\hat{y}$, we have for any $\theta_1, \theta_2$ and any $i$,

$$\ell((\theta_2, x_i), y_i) - \ell((\theta_1, x_i), y_i) \leq \nabla y \ell((\theta_1, x_i), y_i) \cdot (\theta_2 - \theta_1) + \frac{L}{2} (\|\theta_2 - \theta_1\|^2)$$

(137)

Thus, we have

$$F(\theta_2) - F(\theta_1) = \sum_{i=1}^{n} q_i \left[ \ell((\theta_2, x_i), y_i) - \ell((\theta_1, x_i), y_i) \right]$$

$$\leq \sum_{i=1}^{n} q_i \left[ \nabla y \ell((\theta_1, x_i), y_i) \cdot (\theta_2 - \theta_1) + \frac{L}{2} \|\theta_2 - \theta_1\|^2 \right]$$

(138)

which implies that $F(\theta)$ is $L$-smooth.

Denote $\hat{g}(\theta) = \nabla \ell(f(X; \theta), Y) \in \mathbb{R}^n$, then $\nabla F(\theta(t)) = XQ \hat{g}(\theta(t))$, and the update rule is

$$\theta(t+1) = \theta(t) - \eta XQ(t) \hat{g}(\theta(t))$$

(139)

So by the upper quadratic bound, we have

$$F(\theta(t+1)) \leq F(\theta(t)) - \eta(XQ(t) \hat{g}(\theta(t)))^2 + \frac{\eta^2 L}{2} \|XQ(t) \hat{g}(\theta(t))\|^2$$

(140)

Let $\eta_1 = \frac{q^* \lambda_{\text{min}}}{2L(1 + 3\epsilon)\lambda_{\text{max}}}$. Similar to what we did in Appendix D.2.2 (Eqn. (45)), we can prove that for all $\eta \leq \eta_1$, (140) implies that for all $t \geq t_\epsilon$, there is

$$F(\theta(t+1)) \leq F(\theta(t)) - \frac{\eta q^* \lambda_{\text{min}}}{2} \|\sqrt{Q(t)} \hat{g}(\theta(t))\|^2 + \frac{\eta^2 L}{2} \|X \sqrt{Q(t)}\|^2 \|\sqrt{Q(t)} \hat{g}(\theta(t))\|^2$$

$$\leq F(\theta(t)) - \frac{\eta q^* \lambda_{\text{min}}}{4} \|\sqrt{Q(t)} \hat{g}(\theta(t))\|^2 + \frac{\eta^2 L}{2} \|X\|^2 \|\sqrt{Q(t)} \hat{g}(\theta(t))\|^2$$

$$\leq F(\theta(t)) - \frac{\eta q^* \lambda_{\text{min}}}{4} \|\hat{g}(\theta(t))\|^2$$

(141)

This shows that $F(\theta(t))$ is monotonically non-increasing. Since $F(\theta) \geq 0$, $F(\theta(t))$ must converge as $t \to \infty$, and we need to prove that it converges to 0. Suppose that $F(\theta(t))$ does not converge to 0, then there exists a constant $C > 0$ such that
Understand Why Generalized Reweighting Does Not Improve Over ERM

$F(\theta^{(t)}) \geq 2C$ for all $t$. On the other hand, it is easy to see that there exists $\theta^*$ such that $\ell((\theta^*, x_i), y_i) < C$ for all $i$. (141) also implies that $\|\hat{g}(\theta^{(t)})\|_2 \to 0$ as $t \to \infty$ because we must have $F(\theta^{(t)}) - F(\theta^{(t+1)}) \to 0$.

Note that from (139) we have

\[ \|\theta^{(t+1)} - \theta^*\|^2_2 = \|\theta^{(t)} - \theta^*\|^2_2 + 2\eta (X Q^{(t)} \hat{g}(\theta^{(t)}), \theta^* - \theta^{(t)}) + \eta^2 \|X Q^{(t)} \hat{g}(\theta^{(t)})\|^2_2 \] (142)

Denote

\[ F_i(\theta) = \sum_{i=1}^n q_i^{(t)} \ell(\theta, x_i, y_i) \] (143)

Then $F_i$ is convex because $\ell$ is convex and $q_i^{(t)}$ are non-negative, and $\nabla F_i(\theta^{(t)}) = X Q^{(t)} \hat{g}(\theta^{(t)})$. By the lower linear bound $F_i(y) \geq F_i(x) + \langle \nabla F_i(x), y - x \rangle$, we have for all $t$,

\[ \langle X Q^{(t)} \hat{g}(\theta^{(t)}), \theta^* - \theta^{(t)} \rangle \leq F_i(\theta^*) - F_i(\theta^{(t)}) \leq F_i(\theta^*) - \frac{2}{3} F(\theta^{(t)}) \leq C - \frac{4C}{3} = -\frac{C}{3} \] (144)

because $q_i^{(t)} \geq q_i - \epsilon \geq \frac{2}{3} q_i$ and $\sum_{i=1}^n q_i^{(t)} = 1$. Since $\|\hat{g}(\theta^{(t)})\|_2 \to 0$, there exists $T > 0$ such that for all $t \geq T$ and all $\eta \leq \eta_0$,

\[ \|\theta^{(t+1)} - \theta^*\|^2_2 \leq \|\theta^{(t)} - \theta^*\|^2_2 - \frac{2C}{3} \] (145)

which means that $\|\theta^{(t)} - \theta^*\|^2_2 \to -\infty$ because $\frac{2C}{3}$ is a positive constant. This is a contradiction! Thus, $F(\theta^{(t)})$ must converge to 0, which is result (i).

(i) immediately implies (ii) because $\ell$ is strictly decreasing to 0 by condition.

Now let’s prove (iii). First of all, the uniqueness of $\theta_R$ can be easily proved from the convexity of $F(\theta)$. The condition implies that $y_i(\theta_R, x_i) > 0$, i.e., $\theta_R$ must classify all training samples correctly. If there are two different minimizers $\theta_R$ and $\theta_R'$ in whom norm is at most $R$, then consider $\theta''_R = \frac{1}{2}(\theta_R + \theta_R')$. By the convexity of $F$, we know that $\theta''_R$ must also be a minimizer, and $\|\theta''_R\|_2 < R$. Thus, $F(\frac{R}{\|\theta''_R\|_2} \theta''_R) < F(\theta''_R)$ and $\|\frac{R}{\|\theta''_R\|_2} \theta''_R\|_2 = R$, which contradicts with the fact that $\theta''_R$ is a minimizer.

To prove the rest of (iii), the key is to consider (140). On one hand, similar to (41) we can prove that for all $t \geq t_\epsilon$, there is

\[ \left| \langle X Q^{(t)} \hat{g}(\theta^{(t)}), X (Q^{(t)} - Q) \hat{g}(\theta^{(t)}) \rangle \right| \leq \lambda_{\max} \sqrt{3\epsilon} \|\sqrt{Q^{(t)}} \hat{g}(\theta^{(t)})\|^2_2 \] (146)

Since we choose $\epsilon = \min\left\{ \frac{\eta_2^2}{\lambda_{\max}^2}, \left( \frac{\lambda_{\min}}{\lambda_{\max}} \right)^2 \right\}$, this inequality implies that

\[ \|\nabla F_i(\theta^{(t)})\|^2_2 = \|X Q^{(t)} \hat{g}(\theta^{(t)})\|^2_2 \geq \lambda_{\min} \|Q^{(t)} \hat{g}(\theta^{(t)})\|^2_2 \geq \lambda_{\min} (q^* - \epsilon) \|\sqrt{Q^{(t)}} \hat{g}(\theta^{(t)})\|^2_2 \] (147)

On the other hand, if $\eta \leq \eta_2 = \frac{1}{3\epsilon}$, we will have

\[ \frac{\eta^2 L}{2} \|X Q^{(t)} \hat{g}(\theta^{(t)})\|^2_2 \leq \frac{\eta}{4} \|\nabla F_i(\theta^{(t)})\|^2_2 \] (148)

Combining all the above with (140) yields

\[ F(\theta^{(t+1)}) - F(\theta^{(t)}) \leq -\frac{\eta}{2} \|\nabla F_i(\theta^{(t)})\|^2_2 \] (149)

Denote $u = \lim_{R \to \infty} \frac{\theta^*}{\|\theta^*\|_2}$. Similar to Lemma 9 in Ji et al., 2020, we can prove that: for any $\alpha > 0$, there exists a constant $\rho(\alpha) > 0$ such that for any $\theta$ subject to $\|\theta\|_2 \geq \rho(\alpha)$, there is

\[ F_i((1 + \alpha)\|\theta\|_2 u) \leq F_i(\theta) \] (150)
for any $t$. Let $t_\alpha \geq t_e$ satisfy that for all $t \geq t_\alpha$, $\|\theta^{(i)}\|_2 \geq \max \{ \rho(\alpha), 1 \}$. By the convexity of $F_t$, for all $t \geq t_\alpha$,

$$\langle \nabla F_t(\theta^{(i)}), \theta^{(t)} - (1 + \alpha)\|\theta^{(i)}\|_2 u \rangle \geq F_t(\theta^{(i)}) - F_t((1 + \alpha)\|\theta^{(i)}\|_2 u) \geq 0$$

(151)

Thus, we have

$$\langle \theta^{(t+1)} - \theta^{(t)}, u \rangle = -\eta \langle \nabla F_t(\theta^{(t)}), u \rangle \geq \frac{1}{(1 + \alpha)}\|\theta^{(t)}\|_2 - \frac{1}{1 + \alpha} \|\theta^{(t)}\|_2 \geq \frac{1}{(1 + \alpha)}\|\theta^{(t)}\|_2$$

(152)

By $\frac{1}{2}(\|\theta^{(t+1)}\|_2 - \|\theta^{(t)}\|_2)^2 \geq 0$, we have $\frac{1}{2}(\|\theta^{(t+1)}\|_2^2 - \|\theta^{(t)}\|_2^2)/\|\theta^{(t)}\|_2 \geq \|\theta^{(t+1)}\|_2 - \|\theta^{(t)}\|_2$. Moreover, by (149) we have

$$\frac{\|\theta^{(t+1)} - \theta^{(t)}\|_2^2}{2(1 + \alpha)\|\theta^{(t)}\|_2} \leq \frac{\eta^2 \|\nabla F_t(\theta^{(t)}\|_2^2}{2} \leq \eta \left( F(\theta^{(t)}) - F(\theta^{(t+1)}) \right)$$

(153)

Summing up (152) from $t = t_\alpha$ to $t - 1$, we have

$$\langle \theta^{(t)} - \theta^{(t_\alpha)}, u \rangle \geq \frac{\|\theta^{(t)}\|_2^2 - \|\theta^{(t_\alpha)}\|_2^2}{1 + \alpha} + \eta \left( F(\theta^{(t)}) - F(\theta^{(t_\alpha)}) \right) \geq \frac{\|\theta^{(t)}\|_2^2 - \|\theta^{(t_\alpha)}\|_2^2}{1 + \alpha} - \eta F(\theta^{(t_\alpha)})$$

(154)

which implies that

$$\left( \frac{\theta^{(t)}}{\|\theta^{(t)}\|_2}, u \right) \geq \frac{1}{1 + \alpha} \frac{\eta}{\|\theta^{(t)}\|_2} \left( \langle \theta^{(t_\alpha)}, u \rangle - \frac{\|\theta^{(t_\alpha)}\|_2}{1 + \alpha} - \eta F(\theta^{(t_\alpha)}) \right)$$

(155)

Since $\lim_{t \to \infty} \|\theta^{(t)}\|_2 = \infty$, we have

$$\liminf_{t \to \infty} \left( \frac{\theta^{(t)}}{\|\theta^{(t)}\|_2}, u \right) \geq \frac{1}{1 + \alpha}$$

(156)

Since $\alpha$ is arbitrary, we must have $\lim_{t \to \infty} \frac{\theta^{(t)}}{\|\theta^{(t)}\|_2} = u$ as long as $\eta \leq \min \{ \eta_1, \eta_2 \}$.

D.5.3. Corollary of Theorem 5.2

We can show that for the logistic loss, it satisfies all conditions of Theorem 5.2 and $\lim_{R \to \infty} \frac{\theta_B}{R} = \hat{\theta}_{\text{MM}}$. First of all, for the logistic loss we have $\nabla^2 \ell(\hat{y}, y) = \frac{y^2}{e^{\theta x + \epsilon} + e^{-\theta x + \epsilon} + 2} \leq \max \frac{y^2}{2}$, so $\ell$ is smooth.

Then, we prove that $\lim_{R \to \infty} \frac{\theta_B}{R}$ exists and is equal to $\hat{\theta}_{\text{MM}}$. For the logistic loss, it is easy to show that for any $\hat{\theta} \neq \hat{\theta}_{\text{MM}}$, there exists an $\hat{R} > 0$ such that $F(R \cdot \hat{\theta}) > F(R \cdot \hat{\theta}_{\text{MM}})$ for all $\theta \in B(\hat{\theta}, \delta(\hat{\theta}))$.

Let $S = \{ \theta : \|\theta\|_2 = 1 \}$. For any $\epsilon > 0$, $S - B(\hat{\theta}_{\text{MM}}, \epsilon)$ is a compact set. And for any $\theta \in S - B(\hat{\theta}_{\text{MM}}, \epsilon)$, there exist $R(\theta)$ and $\delta(\theta)$ as defined above. Thus, there must exist $\theta_1, \ldots, \theta_m \in S - B(\hat{\theta}_{\text{MM}}, \epsilon)$ such that $S - B(\hat{\theta}_{\text{MM}}, \epsilon) \subseteq \bigcup_{i=1}^m B(\theta_i, \delta(\theta_i))$. Let $R(\epsilon) = \max \{ R(\theta_1), \ldots, R(\theta_m) \}$, then for all $R \geq R(\epsilon)$ and all $\theta \in S - B(\hat{\theta}_{\text{MM}}, \epsilon)$, $F(R \cdot \hat{\theta}) > F(R \cdot \hat{\theta}_{\text{MM}})$, which means that $\frac{\theta_B}{R} \in B(\hat{\theta}_{\text{MM}}, \epsilon)$ for all $R \geq R(\epsilon)$. Therefore, $\lim_{R \to \infty} \frac{\theta_B}{R}$ exists and is equal to $\hat{\theta}_{\text{MM}}$.

Therefore, any GRW satisfying Assumption 1 makes a linear model converge to the max-margin classifier under the logistic loss.
Understanding Why Generalized Reweighting Does Not Improve Over ERM

D.6. Proof of Theorem 5.3

We first consider the regularized linearized neural network $f_{\text{linreg}}^{(t)}$. Since by Proposition D.2 $f^{(0)}(x)$ is sampled from a zero-mean Gaussian process, there exists a constant $M > 0$ such that $|f^{(0)}(x)| < M$ for all $i$ with high probability. Define

$$F(\theta) = \sum_{i=1}^{n} q_i \ell(\theta, \nabla_\theta f^{(0)}(x_i)) + f^{(0)}(x_i), y_i)$$

(157)

Denote $\hat{\theta}_R = \arg\min_{\theta} \{ F(R \cdot \theta) : \|\theta\|_2 \leq 1 \}$. When the linearized neural network is trained by a GRW satisfying Assumption 1 with regularization, since this is convex optimization and the objective function is smooth, we can prove that with a sufficiently small learning rate, as $t \to \infty$, $\theta^{(t)} \to R \cdot \hat{\theta}_R + \theta^{(0)}$ where $R = \lim_{t \to \infty} \|\theta^{(t)} - \theta^{(0)}\|_2$ (which is the minimizer). And define

$$\gamma = \min_{i=1, \ldots, n} y_i \cdot \langle \hat{\theta}_{\text{MM}}, \nabla_\theta f^{(0)}(x_i) \rangle$$

(158)

First, we derive the lower bound of $R$. By Theorem D.7, with a sufficiently large $\tilde{d}$, with high probability $\tilde{R}(f_{\text{linreg}}^{(t)}) < \epsilon$ implies $\tilde{R}(f_{\text{linreg}}^{(t)}) < 2\epsilon$. By the convexity of $\ell$, we have

$$2\epsilon > \frac{1}{n} \sum_{i=1}^{n} \ell(\langle \hat{R}, x_i \rangle + f^{(0)}(x_i), y_i) \geq \log \left( 1 + \exp \left( \frac{1}{n} \sum_{i=1}^{n} \langle R \hat{\theta}_R, x_i \rangle + f^{(0)}(x_i), y_i \rangle \right) \right)$$

$$\geq \log \left( 1 + \exp \left( \frac{1}{n} \sum_{i=1}^{n} R(\hat{\theta}_R, x_i)y_i - M \right) \right)$$

(159)

which implies that $R = \Omega(-\log 2\epsilon)$ for all $\epsilon \in (0, \frac{1}{4})$.

Denote $\delta = \|\hat{\theta}_{\text{MM}} - \hat{\theta}_R\|_2$. Let $\theta' = \frac{\hat{\beta}_{\text{MM}} + \delta}{2}$, then we can see that $\|\theta'\|_2 = \sqrt{1 - \frac{\delta^2}{4}}$. Let $\hat{\theta}' = \frac{\theta'}{\|\theta'\|_2}$. By the definition of $\hat{\theta}_{\text{MM}}$, there exists $j$ such that $y_j \cdot \langle \hat{\theta}', \nabla_\theta f^{(0)}(x_j) \rangle \leq \gamma$, which implies

$$y_j \cdot \langle \hat{\theta}_{\text{MM}} + \hat{\theta}_R \frac{1}{\sqrt{1 - \frac{\delta^2}{4}}}, \nabla_\theta f^{(0)}(x_j) \rangle \leq \gamma$$

(160)

Thus, we have

$$y_j \cdot \langle \hat{\theta}_R, \nabla_\theta f^{(0)}(x_j) \rangle \leq 2\sqrt{1 - \frac{\delta^2}{4}} \gamma - y_j \cdot \langle \hat{\theta}_{\text{MM}}, \nabla_\theta f^{(0)}(x_j) \rangle$$

$$\leq \left( 2\sqrt{1 - \frac{\delta^2}{4}} - 1 \right) \gamma$$

$$\leq \left( 2(1 - \frac{\delta^2}{8}) - 1 \right) \gamma \quad \text{(since } \sqrt{1 - x} \leq 1 - \frac{x}{2})$$

$$= (1 - \frac{\delta^2}{4}) \gamma$$

(161)

On the other hand, we have

$$q_j \log(1 + \exp(-y_j \cdot \langle R \cdot \hat{\theta}_R, \nabla_\theta f^{(0)}(x_j) \rangle - M)) \leq F(R \cdot \hat{\theta}_R)$$

$$\leq F(R \cdot \hat{\theta}_{\text{MM}}) \leq \log(1 + \exp(-R\gamma + M))$$

(162)

which implies that

$$q^* \log \left( 1 + \exp \left( -(1 - \frac{\delta^2}{4})R\gamma - M \right) \right) \leq \log(1 + \exp(-R\gamma + M))$$

(163)
and this leads to

\[ 1 + \exp(-R\gamma + M) \geq \left( 1 + \exp\left(-\frac{\delta^2}{4}R\gamma - M\right) \right)^q \geq 1 + q^\ast \exp\left(-\frac{\delta^2}{4}R\gamma - M\right) \]  

(164)

which is equivalent to

\[-R\gamma + M \geq -(1 - \frac{\delta^2}{4})R\gamma - M + \log(q^\ast) \]

(165)

Thus, we have

\[ \delta = O(R^{-1/2}) = O((-\log 2\epsilon)^{-1/2}) \]  

(166)

So for any test point \( x \), since \( \|\nabla_\theta f^{(0)}(x)\|_2 \leq M_0 \), we have

\[ |(\hat{\theta}_{MM} - \hat{\theta}_R, \nabla_\theta f^{(0)}(x))| \leq \delta M_0 = O((-\log 2\epsilon)^{-1/2}) \]  

(167)

Combined with Theorem D.7, we have: with high probability,

\[ \limsup_{t \to \infty} | R \cdot f_{MM}(x) - f_{\text{lin}}^{(t)}(x) | = O(R \cdot (-\log 2\epsilon)^{-1/2} + \tilde{d}^{-1/4}) \]

(168)

So there exists a constant \( C > 0 \) such that: As \( \tilde{d} \to \infty \), with high probability, for all \( \epsilon \in (0, \frac{1}{4}) \), if \( |f_{MM}(x)| > C \cdot (-\log 2\epsilon)^{-1/2} \), then \( f_{\text{lin}}^{(t)}(x) \) will have the same sign as \( f_{MM}(x) \) for a sufficiently large \( t \). Note that this \( C \) only depends on \( n, q^\ast, \gamma, M \) and \( M_0 \), so it is a constant independent of \( \epsilon \).

Remark. Note that Theorem 5.3 requires Assumption 1 while Theorem 4.6 does not due to the fundamental difference between the classification and regression. In regression the model converges to a finite point. However, in classification, the training loss converging to zero implies that either (i) The direction of the weight is close to the max-margin classifier or (ii) The norm of the weight is very large. Assumption 1 is used to eliminate the possibility of (ii). If the regularization parameter \( \mu \) is sufficiently large, then a small empirical risk could imply a small weight norm. However, in our theorem we do not assume anything on \( \mu \), so Assumption 1 is necessary.

E. A Note on the Proofs in (Lee et al., 2019)

We have mentioned that the proofs in (Lee et al., 2019), particularly the proofs of their Theorem 2.1 and Lemma 1 in their Appendix G, are flawed. In order to fix their proof, we change the network initialization to (11). In this section, we will demonstrate what goes wrong in the proofs in (Lee et al., 2019), and how we manage to fix the proof. For clarity, we are referring to the following version of the paper: https://arxiv.org/pdf/1902.06720v4.pdf.

To avoid confusion, in this section we will still use the notations used in our paper.

E.1. Their Problems

(Lee et al., 2019) claimed in their Theorem 2.1 that under the conditions of our Lemma 4.5, for any \( \delta > 0 \), there exist \( \tilde{D} > 0 \) and a constant \( C \) such that for any \( \tilde{d} \geq \tilde{D} \), with probability at least \( (1 - \delta) \), the gap between the output of a sufficiently wide fully-connected neural network and the output of its linearized neural network at any test point \( x \) can be uniformly bounded by

\[ \sup_{t \geq 0} | f^{(t)}(x) - f_{\text{lin}}^{(t)}(x) | \leq C \tilde{d}^{-1/2} \]  

(claimed)

(169)

where they used the original NTK formulation and initialization in (Jacot et al., 2018):

\[
\begin{align*}
    h^{t+1} & = \frac{W^t}{\sqrt{d_t}} x^t + \beta b^t \\
    x^{t+1} & = \sigma(h^{t+1}) \\
    h^{t+1} & \sim N(0, 1) \\
    b^{t+1} & \sim N(0, 1) \
\end{align*}
\]

(∀l = 0, · · · , L)  

(170)
where \( x_0 = x \) and \( f(x) = h^{L+1} \). However, in their proof in their Appendix G, they did not directly prove their result for the NTK formulation, but instead they proved another result for the following formulation which they called the standard formulation:

\[
\begin{align*}
\{ h_l^{t+1} &= W_l x_l + \beta b_l^t \\
 x_l^{t+1} &= \sigma(h_l^{t+1}) & \text{and} & \{ W_{i,j}^{l(0)} \sim \mathcal{N}(0, \frac{1}{d_l}) \\
 b_l^{t(0)} \sim \mathcal{N}(0, 1) & \} & (\forall l = 0, \cdots, L)
\end{align*}
\] (171)

See their Appendix F for the definition of their standard formulation. In the original formulation, they also included two constants \( \sigma_w \) and \( \sigma_b \) for standard deviations, and for simplicity we omit these constants here. Note that the outputs of the NTK formulation and the standard formulation at initialization are actually the same. The only difference is that the norm of the weight \( W_l \) and the gradient of the model output with respect to \( W_l \) are different for all \( l \).

In their Appendix G, they claimed that if a network with the standard formulation is trained by minimizing the squared loss with gradient descent and learning rate \( \eta' = \eta / \hat{d} \), where \( \eta \) is our learning rate in Lemma 4.5 and also their learning rate in their Theorem 2.1, then (169) is true for this network, so it is also true for a network with the NTK formulation because the two formulations have the same network output. And then they claimed in their equation (S37) that applying learning rate \( \eta' \) to the standard formulation is equivalent to applying the following learning rates

\[
\eta_W' = \frac{d_l}{d_{\text{max}}} \eta \quad \text{and} \quad \eta_b' = \frac{1}{d_{\text{max}}} \eta
\] (172)

to \( W_l \) and \( b_l^t \) of the NTK formulation, where \( d_{\text{max}} = \max\{d_0, \cdots, d_L\} \).

To avoid confusion, in the following discussions we will still use the NTK formulation and initialization if not stated otherwise.

**Problem 1.** Claim (172) is true, but it leads to two problems. The first problem is that \( \eta_W' = O(d_{\text{max}}^{-1}) \) since \( \eta = O(1) \), while their Theorem 2.1 needs the learning rate to be \( O(1) \). Nevertheless, this problem can be simply fixed by modifying their standard formulation as \( h_l^{t+1} = W_l x_l + \beta \sqrt{d_l} b_l^t \) where \( b_l^{t(0)} \sim \mathcal{N}(0, d_l^{-1}) \). The real problem that is non-trivial to fix is that by (172), there is \( \eta_W' = \frac{d_l}{d_{\text{max}}} \eta \). However, note that \( d_0 \) is a constant since it is the dimension of the input space, while \( d_{\text{max}} \) goes to infinity. With that being said, in (172) they were essentially using a very small learning rate for the first layer \( W_0 \) but a normal learning rate for the rest of the layers, which definitely does not match with their claim in their Theorem 2.1.

**Problem 2.** Another big problem is that the proof of their Lemma 1 in their Appendix G is erroneous, and consequently their Theorem 2.1 is unsound as it heavily depends on their Lemma 1. In their Lemma 1, they claimed that for some constant \( M > 0 \), for any two models with the parameters \( \theta \) and \( \tilde{\theta} \) such that \( \theta, \tilde{\theta} \in B(\theta^{(0)}, C_0) \) for some constant \( C_0 \), there is

\[
\| J(\theta) - J(\tilde{\theta}) \|_F \leq \frac{M}{\sqrt{d}} \| \theta - \tilde{\theta} \|_2 \quad \text{(claimed)}
\] (173)

Note that the original claim in their paper was \( \| J(\theta) - J(\tilde{\theta}) \|_F \leq M \sqrt{d} \| \theta - \tilde{\theta} \|_2 \). This is because they were proving this result for their standard formulation. Compared to the standard formulation, in the NTK formulation \( \theta \) is \( \sqrt{d} \) times larger, while the Jacobian \( J(\theta) \) is \( \sqrt{d} \) times smaller. This is also why here we have \( \theta, \tilde{\theta} \in B(\theta^{(0)}, C_0 d^{-1/2}) \) for the NTK formulation. Therefore, equivalently they were claiming (173) for the NTK formulation.

However, their proof of (173) is incorrect. Specifically, the right-hand side of their inequality (S86) is incorrect. Using the notations in our Appendix D.3.3, their (S86) essentially claimed that

\[
\| \alpha_l - \tilde{\alpha}_l \|_2 \leq \frac{M}{\sqrt{d}} \| \theta - \tilde{\theta} \|_2 \quad \text{(claimed)}
\] (174)

for any \( \theta, \tilde{\theta} \in B(\theta^{(0)}, C_0) \), where \( \alpha_l = \nabla_{h_l} h_l^{L+1} \) and \( \tilde{\alpha}_l \) is the same gradient for the second model. Note that their (S86) does not have the \( \sqrt{d} \) in the denominator which appears in (174). This is because for their standard formulation, \( \theta \) is \( \sqrt{d} \)
times smaller than the original NTK formulation, while $\|\alpha^l\|_2$ has the same order in the two formulations because all $h^l$ are the same.

However, it is actually impossible to prove (174). Consider the following counterexample: Since $\theta$ and $\tilde{\theta}$ are arbitrarily chosen, we can choose them such that they only differ in $b_1^l$ for some $1 \leq l < L$. Then, $\|\theta - \tilde{\theta}\|_2 = |b_1 - \tilde{b}_1|$. We can see that $h^{l+1}$ and $\tilde{h}^{l+1}$ only differ in the first element, and $|h_1^{l+1} - \tilde{h}_1^{l+1}| = |\beta(b_1 - \tilde{b}_1)|$. Moreover, we have $W^{l+1} = \tilde{W}^{l+1}$, so there is

$$\alpha^{l+1} - \tilde{\alpha}^{l+1} = \text{diag}(\hat{\sigma}(h^{l+1})) \frac{W^{l+1T}}{\sqrt{d}} \alpha^{l+2} - \text{diag}(\hat{\sigma}(\tilde{h}^{l+1})) \frac{\tilde{W}^{l+1T}}{\sqrt{d}} \tilde{\alpha}^{l+2}$$

$$= \left[ \text{diag}(\hat{\sigma}(h^{l+1})) - \text{diag}(\hat{\sigma}(\tilde{h}^{l+1})) \right] \frac{W^{l+1T}}{\sqrt{d}} \alpha^{l+2} + \text{diag}(\hat{\sigma}(\tilde{h}^{l+1})) \left[ \frac{\tilde{W}^{l+1T}}{\sqrt{d}} (\alpha^{l+2} - \tilde{\alpha}^{l+2}) \right]$$

Then we can lower bound $\|\alpha^{l+1} - \tilde{\alpha}^{l+1}\|_2$ by

$$\|\alpha^{l+1} - \tilde{\alpha}^{l+1}\|_2 \geq \left\| \left[ \text{diag}(\hat{\sigma}(h^{l+1})) - \text{diag}(\hat{\sigma}(\tilde{h}^{l+1})) \right] \frac{W^{l+1T}}{\sqrt{d}} \alpha^{l+2} \right\|_2$$

$$- \left\| \text{diag}(\hat{\sigma}(\tilde{h}^{l+1})) \left[ \frac{\tilde{W}^{l+1T}}{\sqrt{d}} (\alpha^{l+2} - \tilde{\alpha}^{l+2}) \right] \right\|_2 \tag{175}$$

The first term on the right-hand side is equal to $\left[ \hat{\sigma}(h_1^{l+1}) - \hat{\sigma}(\tilde{h}_1^{l+1}) \right] \left\langle W^{l+1T}/\sqrt{d}, \alpha^{l+2} \right\rangle$ where $W_1^{l+1}$ is the first row of $W^{l+1}$. We know that $\|W_1^{l+1}\|_2 = \Theta \left( \sqrt{d} \right)$ with high probability as its elements are sampled from $\mathcal{N}(0, 1)$, and in their (S85) they claimed that $\|\alpha^{l+2}\|_2 = O(1)$, which is true. In addition, they assumed that $\hat{\sigma}$ is Lipschitz. Hence, we can see that

$$\left\| \left[ \text{diag}(\hat{\sigma}(h^{l+1})) - \text{diag}(\hat{\sigma}(\tilde{h}^{l+1})) \right] \frac{W^{l+1T}}{\sqrt{d}} \alpha^{l+2} \right\|_2 = O \left( \left\| \left[ \hat{\sigma}(h_1^{l+1}) - \hat{\sigma}(\tilde{h}_1^{l+1}) \right] \right\|_2 \right)$$

$$= O \left( \left\| h_1^{l+1} - \tilde{h}_1^{l+1} \right\|_2 \right) = O \left( \left\| \theta - \tilde{\theta} \right\|_2 \right) \tag{176}$$

On the other hand, suppose that claim (174) is true, then $\|\alpha^{l+2} - \tilde{\alpha}^{l+2}\|_2 = O \left( \tilde{d}^{-1/2} \left\| \theta - \tilde{\theta} \right\|_2 \right)$. Then we can see that the second term on the right-hand side is $O \left( \tilde{d}^{-1/2} \left\| \theta - \tilde{\theta} \right\|_2 \right)$ because $\|W^{l+1}\|_2 = O(\sqrt{d})$ and $\hat{\sigma}(x)$ is bounded by a constant $\sigma$ is Lipschitz. Thus, for a very large $\tilde{d}$, the second-term is an infinitely small term compared to the first term, so we can only prove that

$$\|\alpha^{l+1} - \tilde{\alpha}^{l+1}\|_2 = O \left( \left\| \theta - \tilde{\theta} \right\|_2 \right) \tag{177}$$

which is different from (174) because it lacks a critical $\tilde{d}^{-1/2}$ and thus leads to a contradiction. Hence, we cannot prove (174) with the $\tilde{d}^{-1/2}$ factor, and consequently we cannot prove (173) with the $\sqrt{d}$ in the denominator on the right-hand side. As a result, their Lemma 1 and Theorem 2.1 cannot be proved without this critical $\tilde{d}^{-1/2}$. Similarly, we can also construct a counterexample where $\theta$ and $\tilde{\theta}$ only differ in the first row of some $W^l$.

**E.2. Our Fixes**

Regarding Problem 1, we can still use an $O(1)$ learning rate for the first layer in the NTK formulation given that $\|x\|_2 \leq 1$. This is because for the first layer, we have

$$\nabla_W \circ f(x) = \frac{1}{\sqrt{d_0}} x^0 \alpha^1^T = \frac{1}{\sqrt{d_0}} x \alpha^1^T \tag{179}$$

For all $l \geq 1$, we have $\|x^l\|_2 = O(\tilde{d}^{1/2})$. However, for $l = 0$, we instead have $\|x^0\|_2 = O(1)$. Thus, we can prove that the norm of $\nabla_W \circ f(x)$ has the same order as the gradient with respect to any other layer, so there is no need to use a smaller learning rate for the first layer.
As a final remark, one key reason why we need to initialize \( W \) is that the dimension of the output space is finite, and in our case it is \( L \). Suppose we allow the dimension of \( h^{L+1} \) to be \( d \) which goes to infinity, then using the same proof techniques, for the NTK formulation we can prove that \( \sup_t \| h^{L+1}(t) - h^{L+1}(t) \|_2 \leq C \), i.e. the gap between two vectors of infinite dimension is always bounded by a finite constant. This is the approximation theorem we need for the infinite-dimensional output space. However, when the dimension of the output space is finite, \( \sup_t \| h^{L+1}(t) - h^{L+1}(t) \|_2 \leq C \) no longer suffices, so we need to decrease the order of the norm of \( W \) in order to obtain a smaller bound.