Early Stopping in Deep Networks: Double Descent and How to Eliminate it

Reinhard Heckel†,* and Fatih Furkan Yılmaz*
†Dept. of Electrical and Computer Engineering, Technical University of Munich
*Dept. of Electrical and Computer Engineering, Rice University
July 21, 2020

Abstract

Over-parameterized models, in particular deep networks, often exhibit a double descent phenomenon, where as a function of model size, error first decreases, increases, and decreases at last. This intriguing double descent behavior also occurs as a function of training epochs, and has been conjectured to arise because training epochs control the model complexity. In this paper, we show that such epoch-wise double descent arises for a different reason: It is caused by a superposition of two or more bias-variance tradeoffs that arise because different parts of the network are learned at different times, and eliminating this by proper scaling of stepsizes can significantly improve the early stopping performance. We show this analytically for i) linear regression, where differently scaled features give rise to a superposition of bias-variance tradeoffs, and for ii) a two-layer neural network, where the first and second layer each govern a bias-variance tradeoff. Inspired by this theory, we study a five-layer convolutional network empirically, and show that eliminating epoch-wise double descent through adjusting stepsizes of different layers improves the early stopping performance significantly.

1 Introduction

Most machine learning algorithms learn a function that predicts a label from features. This function lies in a hypothesis class, such as a neural networks parameterized by its weights. Learning amounts to fitting the parameters of the function by minimizing an empirical risk over the training examples. The goal is to learn a function that performs well on new examples, which are assumed to come from the same distribution as the training examples.

Classical machine learning theory says that the test error or risk as a function of the size of the hypothesis class is U-shaped: a small hypothesis class is not sufficiently expressive to have small error, and a large one leads to overfitting to spurious patterns in the data. The superposition of those two sources of errors, typically referred to as bias and variance, yields the classical U-shaped curve.

However, increasing the model size beyond the number of training examples decreases the error again. This phenomena, dubbed “double descent” by Belkin et al. [Bel+19a] has been observed as early as 1995 by Opper [Opp95], and is highly relevant today because most modern machine learning models, in particular deep neural networks, operate in the over-parameterized regime, where the error decreases again as a function of model size, and where the model is sufficiently expressive to describe any data, even noise.

Interestingly, this double descent behavior also occurs as a function of training time, as observed by Nakkiran et al. [Nak+20] and as illustrated in Figure 1, in particular for learning from noisy labels. The left panel of Figure 1 shows that as a function of training epochs, the test error first decreases, increases, and then decreases again. It is critical to understand this so-called epoch-wise
best early stopping time

Figure 1: **Left:** The test error of an over-parameterized 5-layer convolutional network trained on a noisy version of the CIFAR-10 training set (20% random label noise) as a function of training epochs. As observed by Nakkiran et al. [Nak+20], the performance shows a double descent behavior. **Right:** As we show in this paper, the risk of a regression problem can be decomposed as the sum of two bias-variance tradeoffs. **Both examples:** Early stopping the training where the test error achieves its minima is critical for performance.

double descent behavior to determine the early stopping time that gives the best performance. Early stopping, or other regularization techniques, are critical for learning from noisy labels [Arp+17; YH20].

Nakkiran et al. [Nak+20] conjectured that epoch double descent occurs because the training time controls the “effective model complexity”. This conjecture is intuitive, because the model-size, and thus the size of the hypothesis class, can be controlled by regularizing the empirical risk via early stopping the gradient descent iterations, as formalized in the under-parameterized regime by Yao et al. [Yao+07], Raskutti et al. [Ras+14], and Bühlmann and Yu [BY03]. Specifically, limiting the number of gradient descent iterations ensures that the functions parameters lie in a ball around the initial parameters, and thereby limits the size of the hypothesis class.

In this paper, however, we show empirically and theoretically that epoch-wise double descent arises for a different reason: It is caused by a superposition of bias-variance tradeoffs, as illustrated for a toy-regression example in the right panel of Figure 1. If the risk can be decomposed into two U-shaped bias-variance tradeoffs with minima at different epochs/iterations, then the overall risk/test error has a double descent behavior.

1.1 Contributions

The goal of this paper is to understand the epoch-wise double descent behavior observed by Nakkiran et al. [Nak+20] and depicted in Figure 1. Our main finding is that contrary to model-wise double descent, epoch-wise double descent is not a result of controlling the model complexity with early stopping, but a consequence of a superposition of bias variance tradeoffs. Our contributions are as follows:

- First, we consider a linear regression model and theoretically characterize the risk of early stopped least squares. We show that if features have different scales, then the early stopped
least squares estimate as a function of the early stopping time is a superposition of bias-variance tradeoffs, which yields a double descent like curve. See Figure 1, right panel, as an illustration.

- Second, we characterize the early stopped risk of a two-layer neural network theoretically and show that it is upper bounded by a curve consisting of overlapping bias-variance tradeoffs that are governed by the initializations and stepsizes of the two layers. Specifically, the initialization scales and stepsizes of the weights in the first and second layer determine whether double descent occurs or not.

- Third, we study a five-layer convolutional network empirically and show that—similarly as for the two-layer model—epoch-wise double descent occurs because the convolutional layers (representation layers) are learned faster than the final, fully connected layer, which results in a superposition of bias-variance tradeoffs.

- Finally we show that epoch-wise double descent can be eliminated through adjusting the stepsizes of different coefficients or layers. Epoch-wise double descent should be eliminated by adjusting the stepsizes and/or the initialization, because this translates to better overall performance.

1.2 Related works

There are a large number of works that have studied early stopping theoretically. Intuitively, each step of an iterative algorithm reduces the bias but increases variance. Thus early stopping can ensure that neither bias nor variance are too large. A variety of papers [Yao+07; Ras+14; BY03; Wei+19] formalized this intuition and developed theoretically sound early stopping rules. Those works do not, however, predict that a double descent curve can occur.

A second, more recent line of works, have studied early stopping from a different perspective, namely that of gradient descent fitting different components of a signal or different labels at different speeds. For a linear least squares problem, the data in the direction of singular vectors associated with large singular values is fitted faster than that in the direction of singular vectors associated with small singular values. Li et al. [Li+20] and Arora et al. [Aro+19] have shown that this view explains why neural network often fit clean labels before noisy ones, and Heckel and Soltanolkotabi [HS20b] have used this view to prove that convolutional neural networks provably denoise images.

Next, we note that our theoretical results for neural networks build on a line of works that relate the dynamics of gradient descent to those of an associated linear model or a kernel method in the highly overparameterized regime [Jac+18; Lee+18; Aro+19; Du+18; OS20; Oym+19; HS20b]. We use the same proof strategy as those papers to characterize the early stopping performance of a simple two-layer neural network, but in contrast to those early works, we develop early stopping results and optimize over the weights in the first and second layer, as opposed to only optimizing over the weights in the first layer. That is important, because we want to demonstrate that initialization and stepsize choices of different layers lead to different bias-variance tradeoffs.

Finally, we note that there is an emerging line of works that theoretically establishes double descent behavior as a function of the model complexity (e.g., measured by the number of parameters of the model) for linear regression [Has+19; Bel+19b], for random feature regression [MM19; d’A+20], and for binary linear regression [Den+20]. Yang et al. [Yan+20] explains model-wise
double descent by studying bias and variance separately and through a bell-shaped variance curve. Contrary to epoch-wise double descent studied here, model-wise double descent is not explained in the literature by a superposition of bias-variance tradeoffs.

2 Early-stopped gradient descent for linear least squares

We start by studying the risk of early stopped gradient descent for linear least squares. Our main finding is that the risk as a function of the early stopping time is characterized by a superposition of bias-variance tradeoffs, and if the features have different scales those bias-variance tradeoff curves add up to a double descent shaped risk curve. We also show that the early stopping performance of the estimator can be improved through double descent elimination by scaling the stepsizes associated with the features.

2.1 Data model and risk

Consider a regression problem, and suppose data is generated from a Gaussian linear model as

\[ y = \langle x, \theta^* \rangle + z, \]

where \( x \in \mathbb{R}^d \) is a zero-mean Gaussian feature vector with diagonal co-variance matrix \( \Sigma = \text{diag}(\sigma_1^2, \ldots, \sigma_d^2) \), and \( z \) is zero-mean Gaussian noise with variance \( \sigma^2 \). We are given a training set \( D = \{(x_1, y_1), \ldots, (x_n, y_n)\} \) consisting of \( n \) data points drawn iid from this linear model.

We consider the class of linear estimators parameterized by the vector \( \hat{\theta} \in \mathbb{R}^d \), which is estimated based on the training data \( D \). Such a linear estimator predicts the label associated with a feature vector \( x \) as \( \hat{y} = \langle x, \hat{\theta} \rangle \). The (mean square) risk of this estimator is

\[ R(\hat{\theta}) = \mathbb{E} \left[ (y - \langle x, \hat{\theta} \rangle)^2 \right], \]

where expectation is over an example \((x, y)\) drawn independently (of the training set) from the underlying linear model. The risk of the estimator can be written as a function of the variances of the feature vectors \( \sigma_i^2 \) and of the coefficients of the underlying true linear model, \( \theta^* = [\theta^*_1, \ldots, \theta^*_d] \), as

\[ R(\hat{\theta}) = \sigma^2 + \sum_{i=1}^{d} \sigma_i^2 (\theta^*_i - \hat{\theta}_i)^2. \] (1)

2.2 Early-stopped least squares estimate

We consider the estimate based on early stopping gradient descent on the empirical risk

\[ \hat{R}(\theta) = \|X\theta - y\|_2^2. \]

Here, the matrix \( X \in \mathbb{R}^{n \times d} \) contains the scaled training feature vectors \( \frac{1}{\sqrt{n}}x_1, \ldots, \frac{1}{\sqrt{n}}x_n \) as rows, and \( y = \frac{1}{\sqrt{n}}[y_1, \ldots, y_n] \) are the corresponding scaled responses. We initialize gradient descent with \( \theta^0 = 0 \) and iterate, for \( t = 1, 2, \ldots \)

\[ \theta^{t+1} = \theta^t - \frac{1}{2} \text{diag}(\eta) \nabla \hat{R}(\theta^t), \]
where \( \text{diag}(\eta) \) is the diagonal matrix containing the stepsizes \( \eta_i > 0 \) associated with each of the features as entries. Note that we allow for different stepsizes for all the features. In the following, we study the properties of the estimate obtained by early stopping gradient descent at iteration \( t \), i.e., \( \theta^t \).

### 2.3 Risk of early stopped least squares

The main result of this section is that in the underparameterized regime, where \( d \ll n \), the risk of gradient descent after \( t \) iterations, \( R(\theta^t) \), is very close to

\[
\tilde{R}(\tilde{\theta}^t) := \sigma^2 + \sum_{i=1}^{d} \frac{\sigma^2_i (\theta^t_i)^2 (1 - \eta_i \sigma^2_i)^{2t}}{U_i(t)} + \frac{\sigma^2}{n} (1 - (1 - \eta_i \sigma^2_i)^{t})^2,
\]

as formalized in the theorem below.

**Theorem 1.** Suppose that the stepsizes obey \( \eta_i \leq \frac{1}{\sigma^2_i} \), for all \( i = 1, \ldots, d \). With probability at least \( 1 - \frac{2d - 5 + 2de^{-n/8} - e^{-d} - 2e^{-32}}{\delta} \) over the random training set generated by a linear Gaussian model with parameters \( \theta^* \) and \( \Sigma \), the difference of the early stopped risk and the risk expression in (2) is at most

\[
|R(\theta^t) - \tilde{R}(\tilde{\theta}^t)| \leq c \left( \max_{i} \eta_i^2 \sigma^4_i \frac{d}{n} \left( \| \Sigma \theta^* \|_2^2 + \frac{d}{n} \sigma^2 \log(d) \right) + \frac{\sigma^2}{n} \sqrt{d} \right).
\]

Here, \( c \) is a numerical constant.

Theorem 1 establishes that the risk \( R \) is approximately equal to the risk expression \( \tilde{R} \) which in turn is a superposition of bias-variance tradeoffs. To see the latter, note that the terms \( U_i(t) \) in the risk expression (2) are in general U-shaped as a function of the early stopping time \( t \), because \( \sigma^2_i (\theta^t_i)^2 (1 - \eta_i \sigma^2_i)^{2t} \) decreases in \( t \) and \( \frac{\sigma^2}{n} (1 - (1 - \eta_i \sigma^2_i)^{t})^2 \) increases in \( t \); see Figure 2a for an illustration. The minimum of the individual U-shaped curves \( U_i(t) \) depends on the product of the stepsize and the \( i \)-th features’ variance, \( \eta_i \sigma^2_i \); the larger this product, the earlier (as a function of the number of iterations, \( t \)) the U-shaped curve reaches its minimum. Therefore, if we add up two (or more) such bias-variance tradeoffs with minima at different iterations, the resulting risk curve can have a double descent shape (again, see Figure 2a). This establishes our claim that differently scaled features in linear regression give rise to epoch-wise double descent.

**Improving performance by eliminating double descent:** Epoch-wise double descent can be eliminated by properly scaling the stepsizes associated with each of the features, so that the individual bias-variance tradeoffs overlap at the same point, as formalized by the following proposition:

**Proposition 1.** Pick some optimal early stopping time \( \tilde{t} \geq 1 \). The minimum of the risk expression \( \min_{\eta_1, \ldots, \eta_d} \min_t \tilde{R}(\tilde{\theta}^t) \) is achieved at iteration \( \tilde{t} \) by choosing the stepsizes pertaining to the coefficients as

\[
\eta_i = \frac{1}{\sigma^2_i} \left( 1 - \left( \frac{\sigma^2/n}{\sigma^2_i (\theta^t_i)^2 + \sigma^2/n} \right)^{1/\tilde{t}} \right).
\]
best stopping time

best stopping time

100
101
102
103
104

100
101
102
103
104

100
101
102
103
104

0
0.1
0.2
0.3
0.4

risk

t iterations

a) constant stepsize

b) elimination with diff. stepsizes

c) before & after elimination

Figure 2: a: The “bias-variance” tradeoffs $U_i(t)$ defined in (2) for the parameters $\theta_1^* = 1.5, \sigma_1 = 1, \eta_1 = 0.05$ (bias-variance 1) and for the parameters $\theta_2^* = 10, \sigma_2 = 0.15, \eta_2 = 0.05$ (bias-variance 2), along with their sum (1+2) which determines the risk of the corresponding estimator. b: Same plot, but this time the bias-variance tradeoff is shifted to the left by increasing the stepsize $\eta_2$ according to Proposition 1, so that its minimum overlaps with that of bias-variance tradeoff 1. This eliminates the double descent behavior and gives a better performance of the resulting estimator (a smaller risk or error). c: The resulting risk curves before and after elimination, demonstrating that the minimum of the risk after double descent elimination is smaller than before elimination.

Proposition 1 is proven by showing that if the stepsizes are chosen as specified as above, then the minima of the U-shaped curves $U_i(t)$ occur at the same iteration $t$.

Elimination of double descent is illustrated in Figure 2b, where we choose the stepsizes so that the two U-shaped curves overlap. By eliminating the double descent optimally so that the all individual bias-variance tradeoffs $U_i(t)$ achieve their minima at the same early stopping point $t$, we achieve the lowest overall risk at the optimal early stopping point. Therefore eliminating double descent is critical for optimal performance.

Intuition for the risk expression (2): The appendix contains a proof of Theorem 1. Here we provide intuition why the risk is governed by the risk expression (2). The gradient descent iterates obey

$$\theta^{t+1} - \theta^* = (I - \text{diag}(\eta)X^TX)(\theta^t - \theta^*) + \text{diag}(\eta)X^Tz,$$

where $z = [z_1, \ldots, z_n]$ is the noise. As we formalize below, in the under-parameterized regime where $n \gg d$, we have that $X^TX \approx \Sigma^2$. Therefore the original iterates are close to the iterates $\tilde{\theta}^t$ defined by

$$\tilde{\theta}^{t+1} - \theta^* = (I - \text{diag}(\eta)\Sigma^T\Sigma)(\tilde{\theta}^t - \theta^*) + \text{diag}(\eta)X^Tz.$$  \hspace{1cm} (4)\]

Those iterates are, up to the extra term $\text{diag}(\eta)X^Tz$, equal to the iterates on the population risk $R(\theta)$. Note that in contrast to the literature where it is common to bound the deviation of the original iterates from the iterates on the population risk $[\text{Ras}+14]$, here we control the deviation of the original iterates to the iterates $\tilde{\theta}^t$.\hspace{1cm}
The iterates $\tilde{\theta}^t$ can easily be written out in closed form. To do so, first note that for the recursion $\theta^{t+1} = \alpha \theta^t + \gamma \sum_{i=1}^{t-1} \alpha^i \theta^0 + \gamma \frac{1 - \alpha^t}{1 - \alpha}$, where we used the formula for a geometric series. Using this relation, and that we are starting our iterations at $\theta^0 = 0$, we obtain for the $i$-th entry of $\tilde{\theta}^t$ that

$$\tilde{\theta}_i^t - \theta_i^* = (1 - \eta \sigma_i^2)^t \theta_i^* + \sigma_i \tilde{x}_i^T z \frac{1 - (1 - \eta \sigma_i^2)^t}{\sigma_i^2} ,$$

where $\tilde{x}_i$ is the $i$-th column of $X$ (not the $i$-th example/feature vector!). Next note that $\mathbb{E} [(\tilde{x}_i^T z)^2] \approx \sigma_i \sigma_i$ because the entries of $z$ are $\mathcal{N}(0, \sigma^2)$ distributed, and the entries of $\tilde{x}_i$ are $1/\sqrt{n} \mathcal{N}(0, \sigma_i^2)$ distributed. Using this expectation in the iterates $\tilde{\theta}^t$, and evaluating the risk of those iterates via the formula for the risk given by (1) yields the risk expression (2). The proof of Theorem 1 in the appendix makes this intuition precise by bounding the difference to those expected iterates.

3 Early stopping in two layer neural networks

In this section, we establish a bound on the risk of a two-layer neural network and show that this bound can be interpreted as a super-position of bias-variance tradeoffs, similar to the expression governing the risk of the linear estimator from the previous section. The risk of the two-layer network is governed by two associated kernels pertaining to the first and second layer, and the initialization scale and stepsizes of the weights in the first and second layer determine whether double descent occurs or not. We also show in an experiment that if double descent occurs, it can be eliminated by adapting the stepsizes of the two layers.

Network model: We consider a two-layer neural network with ReLU activation functions and $k$ neurons in the hidden layer:

$$f_{W, v}(x) = \frac{1}{\sqrt{k}} \text{relu}(x^T W) v .$$

(5)

Here, $x \in \mathbb{R}^d$ is the input of the network, $W \in \mathbb{R}^{d \times k}$ are the weights of the first layer and $v \in \mathbb{R}^k$ are the weights of the second layer. Moreover, relu$(z) = \max(z, 0)$ is the rectified linear unit, applied elementwise. See the left panel of Figure 3 for an illustration of this network.

Data model: We assume that we are given a training set $D = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ with examples $(x_i, y_i)$ drawn iid from some joint distribution. For convenience, we assume the datapoints are normalized, i.e., $\|x_i\|_2 = 1$, and that the labels are bounded, i.e., $|y_i| \leq 1$.

Training with early stopped gradient descent: We train the neural network with early stopped and randomly initialized gradient descent on a quadratic loss. We choose the weights at initialization $v^0, W^0$ as

$$[W^0]_{i,j} \sim \mathcal{N}(0, \omega^2), \quad [v^0]_i \sim \text{Uniform}([-\nu, \nu]).$$

(6)

Here, $\omega$ and $\nu$ are parameters that trade off the magnitude of the weights of the first and second layer. Note that with this initialization, for a fixed unit norm $x$, we have $f_{W_0, v_0}(x) = O(\nu \omega)$. We
apply gradient descent to the mean-squared loss
\[ \mathcal{L}(W, v) = \frac{1}{2} \sum_{i=1}^{n} (y_i - f_{W, v}(x_i))^2. \]

The gradient descent updates are \( v_{t+1} = v_t - \eta \nabla_{v} \mathcal{L}(W_t, v_t) \) and \( W_{t+1} = W_t - \eta \nabla_{W} \mathcal{L}(W_t, v_t) \), where \( \eta \) is a constant learning rate. We study the risk of the network as a function of the (early stopped) iterations \( t \).

**Evaluation and performance metric:** Our goal is to bound the test error as a function of the iterations of gradient descent. Let \( \ell: \mathbb{R} \times \mathbb{R} \to [0,1] \) be a loss function that is 1-Lipschitz in its first argument and obeys \( \ell(y, y) = 0 \); a concrete example is the loss \( \ell(z, y) = |z - y| \) for arguments \( z, y \in [0,1] \). The test error or risk is defined, as before, as
\[ R(f) = \mathbb{E} [\ell(f(x), y)], \]
where expectation is over examples \((x, y)\) drawn from the unknown joint distribution from which the training set is drawn as well. Note that we train on the least squares loss, but we test in terms of the risk defined above.

### 3.1 Risk of early stopped neural network training

Our main result is a bound on the test error of the two layer neural network trained for \( t \) iterations. The result depends on the Gram matrix \( \Sigma \in \mathbb{R}^{n \times n} \) defined by two kernels associated with the first and second layer of the network. The \((i,j)\)-th entry of the Gram matrix as a function of the training examples is defined as
\[ \Sigma_{ij} = \nu^2 K_1(x_i, x_j) + \omega^2 K_2(x_i, x_j), \quad (7) \]
with kernels
\[
K_1(x_i, x_j) = \frac{1}{2} \left( 1 - \frac{\cos^{-1}(\rho_{ij})}{\pi} \right) \rho_{ij} \\
K_2(x_i, x_j) = \frac{1}{2} \left( \frac{\sqrt{1 - \rho_{ij}^2}}{\pi} + \left( 1 - \frac{\cos^{-1}(\rho_{ij})}{\pi} \right) \rho_{ij} \right)
\]
where \( \rho_{ij} = \langle \mathbf{x}_i, \mathbf{x}_j \rangle \) (recall that we assume \( \| \mathbf{x}_i \|_2 = 1 \), for all \( i \)). See Figure 3 for a plot of the kernels as a function of \( \rho_{ij} \). Our result depends on the singular values and vectors of this Gram matrix:

\[
\Sigma = \sum_{i=1}^{n} \sigma_i^2 \mathbf{u}_i \mathbf{u}_i^T.
\]

We are now ready to state our result.

**Theorem 2.** Let \( \alpha > 0 \) be the smallest eigenvalue of the Gram matrix \( \Sigma \), and suppose that the network is sufficiently wide, i.e., \( k \geq \Omega \left( \frac{n^{10}}{\alpha^{14} \min(\nu, \omega)} \right) \), and suppose the initialization scale parameters obey \( \nu \omega \leq \alpha / \sqrt{32 \log(2n/\delta)} \) and \( \nu + \omega \leq 1 \) for some \( \delta \in (0, 1) \). Then, with probability at least \( 1 - \delta \), the risk of the network trained with gradient descent for \( t \) iterations is at most

\[
R(f_{W_t, \nu_t}) \leq \sqrt{\frac{1}{n} \sum_{i=1}^{n} \langle \mathbf{u}_i, \mathbf{y} \rangle^2 (1 - \eta \sigma_i^2)^{2t}} + \frac{1}{n} \sum_{i=1}^{n} \langle \mathbf{u}_i, \mathbf{y} \rangle^2 \frac{(1 - (1 - \eta \sigma_i^2)^t)^2}{\sigma_i^2} + O(1/\sqrt{n}). \quad (8)
\]

Regarding the assumptions of the theorem, we remark that the exponent of \( n \) and \( \alpha \) in the width-condition \( (k \geq \Omega \left( \frac{n^{10}}{\alpha^{14} \min(\nu, \omega)} \right) ) \) can be improved. Regarding the assumption that the smallest eigenvalue of the Gram matrix obeys \( \alpha > 0 \), Theorem 3.1 by Du et al. [Du+19] shows that if no two \( \mathbf{x}_i, \mathbf{x}_j \) are parallel, then \( \alpha > 0 \), for a very related Gram matrix. As argued in that work, for most real-world datasets no two inputs are parallel, therefore the assumption on the Gram matrix is rather mild.

Note that the risk bound established by Theorem 2 can be interpreted as a superposition of \( n \)-many bias variance tradeoffs, similar to the expression (2) governing the risk of early stopped linear least squares. Specifically, the \( i \)-th “bias” term \( \langle \mathbf{u}_i, \mathbf{y} \rangle^2 (1 - \eta \sigma_i^2)^{2t} \) decreases in the number of gradient descent iterations \( t \), while the \( i \)-th “variance” term \( \langle \mathbf{u}_i, \mathbf{y} \rangle^2 \frac{(1 - (1 - \eta \sigma_i^2)^t)^2}{\sigma_i^2} \) increases in the number of gradient descent iterations. The speed at which the bias and variance terms corresponding to the \( i \)-th singular value increase and decrease, respectively, depends on the singular value \( \sigma_i^2 \). Those singular values, in turn, are determined by the kernels \( K_1 \) and \( K_2 \), the random initialization (in particular the scale parameters \( \nu, \omega \)), and the distribution of the examples.

Whether epoch-wise double descent occurs or not depends on those singular values and therefore on the kernels, the initialization, and the distribution of the examples. In Figure 4, we depict the of the two layer network trained on data drawn from a linear model for different initialization parameters \( \omega, \nu \), and observe this dependence.

**Improving performance by eliminating double descent:** Similarly as for the linear least squares problem studied in the previous section, it is possible to shape the bias variance tradeoffs by adapting the stepsizes (or through initialization of the layers). However, this is not as straightforward as for the linear-least square problem with **diagonal covariance matrix** studied in the previous section because changing the stepsize of one weight can impact all other weight updates.

Nevertheless, we can change the stepsizes pertaining to the different layers and thereby control whether we do or do not have double descent. To see why, suppose we choose the initialization equally, i.e., \( \omega = 1 \) and \( \nu = 1 \), but update the variables of the second layer (i.e., \( \mathbf{v} \)) with a much larger stepsize than those of the first layer (i.e., \( \mathbf{W} \)). Then the kernel associated with the second
Figure 4: Risk of the two-layer neural network trained on data drawn from a linear model with diagonal covariance matrix with geometrically decaying variances. The weights in the first and second layer are randomly initialized with scale parameters $\omega$ and $\nu$ and the network is trained by minimizing the least-squares loss with gradient descent. The results show that the empirical risk computed on an independent test set has a double descent shape. Moreover, choosing a smaller stepsize for the weights in the second layer eliminates the double descent and improves the risk performance as suggeste by the theory.

layer dominates and the network behaves like a random feature model [RR08]. Similarly, if we update the variables of the first layer (i.e., $W$) with a much larger stepsize than those of the second layer (i.e., $W$) then the network behaves like a network with the final layer weights $v$ fixed. Thus, the stepsizes trade off the impact of the two kernels, and this tradeoff yields overlapping bias-variance tradeoffs and therefore a double descent curve.

In Figure 4, we illustrate this behavior. We consider data drawn from a linear model, specifically, we draw data from the linear model specified in Section 2.1 with geometrically decaying diagonal co-variance entries $\sigma_i$ and zero additive noise, i.e., $\sigma = 0$. We then train the network for different initialization scale parameters $\omega, \nu$ once with the same stepsize $\eta = 8e^{-5}$, and once with a smaller stepsize for the first layer, i.e., $\eta_W = 1e^{-6}$ and $\eta_v = 8e^{-5}$. It can be seen that the empirical risk has a double-descent behavior for $\omega = \nu = 1$ and when using the same stepsize for both layers. Moreover, double descent is eliminated by choosing a smaller stepsize for the first layer, or by choosing a smaller initialization for the first layer, as suggested by our theoretical results, and similar to the linear least squares setup as discussed in the previous section. Also note that, not only does choosing a smaller stepsize for the first layer eliminate double descent, it also gives a better overall risk.

4 Early stopping in convolutional neural networks

Here, we study the risk of training a standard 5-layer convolutional neural network (CNN) on the (10 class) CIFAR-10 dataset. This network was studied in [Nak+20], and we note that, as shown in that paper, the risk (or test error) only has a double descent behavior if the network is trained on a dataset with label noise. In this section we consider the same setup and train on the CIFAR-10 training set with 20% random label noise. We show—inspired by our theory—that epoch-wise
Figure 5: Mitigating double descent for a 5-layer CNN trained on noisy CIFAR-10. **Left:** The Frobenius norm of the Jacobian associated with the convolutional layer and the fully connected layer across training iterations. **Right:** Test error of the CNN trained with the i) same stepsize for all layer, and with ii) a smaller stepsize for the last fully connected layer. Decreasing the learning rate of the last layer causes the last layer to be learned at a similar speed as the convolutional layers and thereby eliminates double descent and increases the best early stopped performance (i.e., the minima of ii is smaller than that of i).

double descent can be eliminated and the early stopping performance can be improved by adjusting the stepsizes/learning rates.

To see the intuition behind this approach, recall that the epoch-wise double descent phenomenon in the least squares problem from section 2 stems from the model fitting differently scaled features at different rates. In the two-layer wide neural network from the previous section, the singular values of the Gram matrix play the role of the scaling of the features in the linear model. In the five layer CNN studied here, the corresponding singular values that are (to a large part) associated with the fully connected layer are almost two orders of magnitude larger than those (to a large part) associated with the convolutional layers (see Figure 5). This causes the convolutional layers to be learned slower than the fully connected layer which results in double descent.

To see this effect and to demonstrate its elimination/mitigation, see Figure 5: by decreasing the stepsize of the weights associated with the fully connected layer, the convolutional and fully connected layers are learned at a similar speed which eliminates the double descent behavior and increases the performance (the test error of “ii: smaller stepsize fully connected layer” is smaller than that of “i: same stepsize”).

We next demonstrate that the singular values (largely) associated with the fully connected layer are almost two orders of magnitude larger than those (largely) associated with the convolutional layers. We say “largely associated” because the individual singular values are not only associated with a single layer or single weights, but some of the singular values are dominated by the convolutional layers and others by the fully connected one. To make this more precise, let $\theta^t$ be the weights of the network at iteration or epoch $t$, and let $f(\theta^t) = [f_{\theta^t}(x_1), \ldots, f_{\theta^t}(x_n)]$ be the predictions of the network with weights $\theta^t$. Here, $f_{\theta^t}(x)$ is the prediction of the network for image (input) $x$. Let
$\mathbf{J}_{C,k}$ and $\mathbf{J}_{F,k}$ be the Jacobian matrices of the networks predictions $f(\theta^t)$ at iteration $t$ pertaining to the weights in the convolutional and the weights of the fully connected layers, respectively. The networks’ dynamics are determined by the Jacobians $\mathbf{J}_{C,k}$ and $\mathbf{J}_{F,k}$. To measure whether the singular values largely associated with the different layers vary significantly, which can give rise to double descent (per the previous section), we plot in Figure 5 the squared Frobenius norms of $\mathbf{J}_{C,k}$ and $\mathbf{J}_{F,k}$, and observe that $\|\mathbf{J}_{F,k}\|_F^2$ (fully connected layer) is by two orders of magnitude larger than $\|\mathbf{J}_{C,k}\|_C^2$ (convolutional layers). To see the connection to singular values, recall that the squared Frobenius norm of a matrix is the sum of its singular values.

To make the connection to the previous section more explicit, note that the Gram matrix at initialization is given by $\Sigma_0 = [\mathbf{J}_{C,0} \mathbf{J}_{F,0}] [\mathbf{J}_{C,0}^T \mathbf{J}_{F,0}^T]$. The Gram matrix of the finite-width network is iteration dependent, because the network does not operate in the infinite-width limit. However, as Figure 5 shows, its norm changes moderately over the iterations, and the relative scale of the two terms is mostly preserved.

**Code**

Code to reproduce the experiments is available at [https://github.com/MLI-lab/early_stopping_double_descent](https://github.com/MLI-lab/early_stopping_double_descent).

**Acknowledgements**

R. Heckel and F. F. Yilmaz are (partially) supported by NSF award IIS-1816986. R. Heckel acknowledges support of the NVIDIA Corporation in form of a GPU, and would like to thank Fanny Yang and Alexandru Tifrea for discussions and helpful comments on this manuscript.

**References**

[Aro+19] S. Arora, S. Du, W. Hu, Z. Li, and R. Wang. “Fine-Grained Analysis of Optimization and Generalization for Overparameterized Two-Layer Neural Networks”. In: *International Conference on Machine Learning*. 2019, pp. 322–332.

[Arp+17] D. Arpit et al. “A Closer Look at Memorization in Deep Networks”. In: *International Conference on Machine Learning*. 2017, pp. 233–242.

[Bel+19a] M. Belkin, D. Hsu, S. Ma, and S. Mandal. “Reconciling Modern Machine-Learning Practice and the Classical Bias–Variance Trade-Off”. In: *Proceedings of the National Academy of Sciences* 116.32 (2019), pp. 15849–15854.

[Bel+19b] M. Belkin, D. Hsu, and J. Xu. “Two Models of Double Descent for Weak Features”. In: *arXiv:1903.07571 [cs, stat]* (2019).

[BY03] P. Bühlmann and B. Yu. “Boosting With the L2 Loss”. In: *Journal of the American Statistical Association* 98.462 (2003), pp. 324–339.

[Dan+16] A. Daniely, R. Frostig, and Y. Singer. “Toward Deeper Understanding of Neural Networks: The Power of Initialization and a Dual View on Expressivity”. In: *Advances in Neural Information Processing Systems 29*. 2016, pp. 2253–2261.
[d’A+20] S. d’Ascoli, M. Refinetti, G. Biroli, and F. Krzakala. “Double Trouble in Double Descent: Bias and Variance(s) in the Lazy Regime”. In: *International Conference on Machine Learning*. 2020.

[Den+20] Z. Deng, A. Kammoun, and C. Thrampoulidis. “A Model of Double Descent for High-Dimensional Binary Linear Classification”. In: *arXiv:1911.05822 [cs, eess, stat]* (2020).

[Du+19] S. Du, J. Lee, H. Li, L. Wang, and X. Zhai. “Gradient Descent Finds Global Minima of Deep Neural Networks”. In: *International Conference on Machine Learning*. 2019, pp. 1675–1685.

[Du+18] S. S. Du, X. Zhai, B. Poczos, and A. Singh. “Gradient Descent Provably Optimizes Over-Parameterized Neural Networks”. In: *International Conference on Learning Representations*. 2018.

[FR13] S. Foucart and Rauhut, Holger. *A Mathematical Introduction to Compressive Sensing*. Springer Berlin Heidelberg, 2013.

[Has+19] T. Hastie, A. Montanari, S. Rosset, and R. J. Tibshirani. “Surprises in High-Dimensional Ridgeless Least Squares Interpolation”. In: *arXiv:1903.08560 [cs, math, stat]* (2019).

[HS20a] R. Heckel and M. Soltanolkotabi. “Compressive Sensing with Un-Trained Neural Networks: Gradient Descent Finds the Smoothest Approximation”. In: *International Conference on Machine Learning*. 2020.

[HS20b] R. Heckel and M. Soltanolkotabi. “Denoising and Regularization via Exploiting the Structural Bias of Convolutional Generators”. In: *International Conference on Learning Representations*. 2020.

[Jac+18] A. Jacot, F. Gabriel, and C. Hongler. “Neural Tangent Kernel: Convergence and Generalization in Neural Networks”. In: *Advances in Neural Information Processing Systems*. 2018, pp. 8571–8580.

[Lee+18] J. Lee, Y. Bahri, R. Novak, S. S. Schoenholz, J. Pennington, and J. Sohl-Dickstein. “Deep Neural Networks as Gaussian Processes”. In: *International Conference on Learning Representations*. 2018.

[Li+20] M. Li, M. Soltanolkotabi, and S. Oymak. “Gradient Descent with Early Stopping Is Provably Robust to Label Noise for Overparameterized Neural Networks”. In: *International Conference on Artificial Intelligence and Statistics*. 2020.

[MM19] S. Mei and A. Montanari. “The Generalization Error of Random Features Regression: Precise Asymptotics and Double Descent Curve”. In: *arXiv:1908.05355 [math, stat]* (2019).

[Moh+12] M. Mohri, A. Rostamizadeh, and A. Talwalkar. *Foundations of Machine Learning*. MIT Press, 2012.

[Nak+20] P. Nakkiran, G. Kaplun, Y. Bansal, T. Yang, B. Barak, and I. Sutskever. “Deep Double Descent: Where Bigger Models and More Data Hurt”. In: *International Conference on Learning Representations*. 2020.

[Opp95] M. Opper. “Statistical Mechanics of Learning: Generalization”. In: *The Handbook of Brain Theory and Neural Networks*. 1995, pp. 922–925.

13
In this section we provide further numerical results for linear least squares. We consider a linear model with $d = 700$ features, and with $n = 6d$ examples. We let a fraction $6/7$ of the features have singular value $\sigma_i = 1$ and associated model coefficient $\theta_i = 1$, and the rest, $1/7$ of the features, have singular value $\sigma_i = 0.1$ and $\theta_i = 10$. In Figure 6(a) we show the risk obtained by simulating the risk empirically along with the risk expression $\bar{R}(\tilde{\theta}_t)$ given by equation (2). It can be seen that the risk expression $\bar{R}(\tilde{\theta}_t)$ slightly under estimates the true risk. The quality of the estimate becomes better as we increase $n$; in Figure 6(b) we show simulations for the same configuration but with $n = 10d$.

B Proof of Theorem 1

The difference of the risk and risk expression can be bounded by

$$\left| R(\theta^t) - \bar{R}(\tilde{\theta}_t) \right| \leq \left| R(\theta^t) - R(\bar{\theta}^t) \right| + \left| R(\bar{\theta}^t) - \bar{R}(\tilde{\theta}_t) \right|. \quad (9)$$

We bound the two terms on the right-hand-side separately. We start with bounding the first term with the lemma below.
Figure 6: The risk of early-stopped gradient least-squares $R(\tilde{\theta}^t)$ based on numerical simulation of the Gaussian model along with the risk expression $\bar{R}(\tilde{\theta}^t)$ given in (2). We averaged over 100 runs of gradient descent, and the shaded region corresponds to one standard deviation over the runs. It can be seen that the risk expression slightly underestimates the true risk, but other than that describes the behavior of the risk well.

**Lemma 1.** Define $\tilde{X}$ so that $X = \tilde{X}\Sigma$. Suppose that $\|I - \tilde{X}^T\tilde{X}\| \leq \epsilon$, with $\epsilon \leq \frac{\min_i \eta_i \sigma_i^2}{2 \max_i \eta_i \sigma_i^2}$. Then

$$\left| R(\theta^t) - R(\tilde{\theta}^t) \right| \leq (1 - (1 - \min_i \eta_i \sigma_i^2 / 2)^t)^{1/2} \max_i \eta_i \sigma_i^4 \epsilon^2 \max_{\ell \in \{1, \ldots, k\}} \|\Sigma \tilde{\theta}^\ell - \Sigma \theta^*\|_2^2.$$  

In order to apply the lemma, we start by verifying its condition. Towards this goal, consider the matrix $X = \tilde{X}\Sigma$ and note that the entries of $\tilde{X}$ are iid $\mathcal{N}(0, 1/n)$. A standard concentration inequality from the compressive sensing literature (e.g., [FR13, Chapter 9]) states that, for any $\beta > 0$,

$$P \left[ \|I - \tilde{X}^T\tilde{X}\| \geq \beta \right] \leq e^{-\frac{n\beta^2}{15d} + 4d}.$$  

With $\beta = \sqrt{\frac{75d}{n}}$ we obtain that, with probability at least $1 - e^{-d}$,

$$\|I - \tilde{X}^T\tilde{X}\| \leq \sqrt{\frac{75d}{n}}.$$  

Next, we bound the term on the RHS of in (10), with the following lemma.

**Lemma 2.** Provided that $\eta_i \sigma_i^2 \leq 1$ for all $i$, with probability at least $1 - 2d(e^{-\beta^2/2} + e^{-n/8})$,

$$\max_{\ell} \|\Sigma \tilde{\theta}^\ell - \Sigma \theta^*\|_2^2 \leq 2\|\Sigma \theta^*\|_2^2 + 4\frac{d}{n}\sigma^2 \beta^2.$$  

Applying the lemma with $\beta^2 = 10 \log(d)$, we obtain that with probability at least $1 - 2d^{-5} + 2de^{-n/8} - e^{-d}$ we have

$$\left| R(\theta^t) - R(\tilde{\theta}^t) \right| \leq 8 \max_i \eta_i^2 \sigma_i^4 \frac{75d}{\min_i \eta_i \sigma_i^2} \left( \frac{2\|\Sigma \theta^*\|_2^2 + 4\frac{d}{n}\sigma^2 10 \log(2d)}{n} \right).$$  

We are now ready to bound the second term in (9):
Lemma 3. With probability at least \(1 - 4e^{-\frac{\beta^2}{8}}\), we have that
\[
\left| R(\tilde{\theta}^t) - \bar{R}(\tilde{\theta}^t) \right| \leq \sigma^2_n \beta 3\sqrt{d},
\] (12)
with \(\bar{R}(\tilde{\theta}^t)\) as defined in (2).

Applying the two bounds (11) and (12) to the RHS of the bound (9) concludes the proof. The remainder of the proof is devoted to proving the three lemmas above.

B.1 Proof of Lemma 1

Recall that the iterates of the original and closely related problem are given by
\[
\begin{align*}
\theta^{t+1} - \theta^* &= (I - \text{diag}(\eta)X^TX)(\theta^t - \theta^*) + \text{diag}(\eta)X^T z, \\
\tilde{\theta}^{t+1} - \theta^* &= (I - \text{diag}(\eta)\Sigma^T \Sigma)(\tilde{\theta}^t - \theta^*) + \text{diag}(\eta)X^T z.
\end{align*}
\]

Note that \(X = \hat{X}\Sigma\), where we defined \(\hat{X}\) which has iid Gaussian entries \(\mathcal{N}(0, 1/n)\). With this notation, and using that \(\Sigma\) is diagonal and therefore commutes with diagonal matrices, we obtain the following expressions for the residuals of the two iterates:
\[
\begin{align*}
\Sigma \theta^{t+1} - \Sigma \theta^* &= (I - \text{diag}(\eta)\Sigma^2 \hat{X}^T \hat{X})(\Sigma \theta^t - \Sigma \theta^*) + \text{diag}(\eta)\Sigma^2 \hat{X}^T z, \\
\Sigma \tilde{\theta}^{t+1} - \Sigma \theta^* &= (I - \text{diag}(\eta)\Sigma^2)(\Sigma \tilde{\theta}^t - \Sigma \theta^*) + \text{diag}(\eta)\Sigma^2 \hat{X}^T z.
\end{align*}
\]

The difference between the residuals is
\[
\begin{align*}
\Sigma \theta^{t+1} - \Sigma \tilde{\theta}^{t+1} &= (I - \text{diag}(\eta)\Sigma^2 \hat{X}^T \hat{X})(\Sigma \theta^t - \Sigma \theta^*) - (I - \text{diag}(\eta)\Sigma^2)(\Sigma \tilde{\theta}^t - \Sigma \theta^*) \\
&= \Sigma \theta^t - \Sigma \tilde{\theta}^t - \text{diag}(\eta)\Sigma^2 \hat{X}^T \hat{X}(\Sigma \theta^t - \Sigma \theta^*) + \text{diag}(\eta)\Sigma^2(\Sigma \tilde{\theta}^t - \Sigma \theta^*), \\
&= (I - \text{diag}(\eta)\Sigma^2 \hat{X}^T \hat{X})(\Sigma \theta^t - \Sigma \theta^*) + \text{diag}(\eta)\Sigma^2(I - \hat{X}^T \hat{X})(\Sigma \tilde{\theta}^t - \Sigma \theta^*),
\end{align*}
\]

where the last inequality follows by adding and subtracting \(\text{diag}(\eta)\Sigma^2 \hat{X}^T \hat{X}(\Sigma \tilde{\theta}^t - \Sigma \theta^*)\) and rearranging the terms. It follows that
\[
\left\| \Sigma \theta^{t+1} - \Sigma \tilde{\theta}^{t+1} \right\|_2 \leq (1 - \min_i \eta_i \sigma_i^2 / 2) \left\| \Sigma \theta^t - \Sigma \tilde{\theta}^t \right\|_2 + \max_i \eta_i \sigma_i^2 \epsilon \max_\ell \left\| \Sigma \tilde{\theta}^\ell - \Sigma \theta^* \right\|_2. \tag{13}
\]

Here, we used the bound
\[
\|I - \text{diag}(\eta)\Sigma^2 \hat{X}^T \hat{X}\| \leq \|I - \text{diag}(\eta)\Sigma^2\| + \|\text{diag}(\eta)\Sigma^2(I - \hat{X}^T \hat{X})\| \leq (1 - \min_i \eta_i \sigma_i^2) + \max_i \eta_i \sigma_i^2 \epsilon \leq (1 - \min_i \eta_i \sigma_i^2 / 2).
\]

Here, the last inequality follows by the assumption \(\epsilon \leq \frac{\min_i \eta_i \sigma_i^2}{2 \max_i \eta_i \sigma_i^2}\). Iterating the bound (13) yields
\[
\left\| \Sigma \theta^t - \Sigma \tilde{\theta}^t \right\|_2 \leq \frac{1 - (1 - \min_i \eta_i \sigma_i^2 / 2)^t}{\min_i \eta_i \sigma_i^2 / 2} \max_i \eta_i \sigma_i^2 \epsilon \max_\ell \left\| \Sigma \tilde{\theta}^\ell - \Sigma \theta^* \right\|_2,
\]
which concludes the proof.
B.2 Proof of Lemma 2

Recall that

\[ \sigma_i(\hat{\theta}_i^t - \theta_i^*) = \sigma_i(1 - \eta_i \sigma_i^2)\theta_i^* + \tilde{x}_i^T z(1 - (1 - \eta_i \sigma_i^2)\theta_i^*). \]

With \( \eta_i \sigma_i^2 \leq 1 \), by assumption, it follows that

\[ \sigma_i^2(\hat{\theta}_i^t - \theta_i^*)^2 \leq 2\sigma_i^2(\theta_i^*)^2 + 2(\tilde{x}_i^T z)^2. \tag{14} \]

Conditioned on \( z \), the random variable \( \tilde{x}_i^T z \) is zero-mean Gaussian with variance \( \|z\|_2/n \). Thus, \( \Pr[|\tilde{x}_i^T z|^2 \geq \frac{\|z\|_2^2}{n} \beta^2] \leq 2e^{-\beta^2/2} \). Moreover, as used previously in (16), with probability at least \( 1 - 2e^{-n/8} \), \( \|z\|_2^2 \leq 2\sigma^2 \). Combining the two with the union bound, we obtain

\[ \Pr[|\tilde{x}_i^T z|^2 \geq \frac{2\sigma^2}{n} \beta^2] \leq 2e^{-\beta^2/2} + 2e^{-n/8}. \]

Using this bound in inequality (14), we have that, with probability at least \( 1 - 2(e^{-\beta^2/2} + e^{-n/8}) \) that

\[ \sigma_i^2(\hat{\theta}_i^t - \theta_i^*)^2 \leq 2\sigma_i^2(\theta_i^*)^2 + \frac{1}{n} \sigma^2 \beta^2. \]

By the union bound over all \( i \) we therefore get that

\[ \max_i \left\| \Sigma \hat{\theta}_i^t - \Sigma \theta_i^* \right\|_2^2 \leq 2\|\Sigma \theta_i^*\|_2^2 + 4\frac{d}{n} \sigma^2 \beta^2, \]

with probability at least \( 1 - 2d(e^{-\beta^2/2} + e^{-n/8}) \).

B.3 Proof of Lemma 3

We have

\[ R(\hat{\theta}) = \sigma^2 + \sum_{i=1}^d \sigma_i^2 \left( (1 - \eta_i \sigma_i^2)\theta_i^* + \sigma_i \tilde{x}_i^T z \frac{1 - (1 - \eta_i \sigma_i^2)\theta_i^*}{\sigma_i^2} \right)^2 \]

\[ = \sigma^2 + \sum_{i=1}^d \left( \sigma_i(1 - \eta_i \sigma_i^2)\theta_i^* + \tilde{x}_i^T z(1 - (1 - \eta_i \sigma_i^2)\theta_i^*) \right)^2. \]

The random variable \( Z_i \), conditioned on \( z \), is a squared Gaussian with variance upper bounded by \( \frac{\|z\|_2^2}{n} \) and has expectation

\[ \mathbb{E}[Z_i] = \sigma_i^2(1 - \eta_i \sigma_i^2)^2(\theta_i^*)^2 + \frac{\|z\|_2^2}{n}(1 - (1 - \eta_i \sigma_i^2)^2) \]

By a standard concentration inequality of sub-exponential random variables, we get, for \( \beta \in (0, \sqrt{d}) \) and conditioned on \( z \), that the event

\[ \mathcal{E}_1 = \left\{ \left| \sum_{i=1}^d (Z_i - \mathbb{E}[Z_i]) \right| \leq \frac{\|z\|_2^2}{n} \sqrt{\beta d} \right\} \]

(15)
occurs with probability at least $1 - 2e^{-\beta^2/\bar{\sigma}^2}$. With the same standard concentration inequality for sub-exponential random variables, we have that the event

$$ E_2 = \left\{ \left| \|z\|_2^2 - \sigma^2 \right| \leq \frac{\sigma^2 \beta}{\sqrt{n}} \right\} $$

also occurs with probability at least $1 - 2e^{-\beta^2/\bar{\sigma}^2}$. By the union bound, both events hold simultaneously with probability at least $1 - 4e^{-\beta^2/\bar{\sigma}^2}$. On both events, we have that

$$ \left| R(\hat{\theta}_t) - \bar{R}(\hat{\theta}^*) \right| \leq \sum_{i=1}^{d} \left( Z_i - \mathbb{E}[Z_i] \right) + \frac{1}{n} \left( \|z\|_2^2 - \sigma^2 \right) \left( 1 - (1 - \eta_i \sigma_i^2)^t \right)^2 $$

$$ \leq \sum_{i=1}^{d} \left( Z_i - \mathbb{E}[Z_i] \right) + d \|z\|_2^2 - \sigma^2 $$

$$ \leq \frac{\|z\|_2^2}{n} \sqrt{d \beta} + \frac{d}{n} \frac{\sigma^2}{\sqrt{n}} $$

$$ \leq \frac{2\sigma^2}{n} \sqrt{d \beta} + \frac{d}{n} \frac{\sigma^2}{\sqrt{n}} $$

$$ \leq \frac{\sigma^2}{n} \beta \sqrt{d}, $$

concluding the proof of our lemma.

### C Proof of Proposition 1

By equation (2), the risk expression is a sum of U-shaped curves: $R(\hat{\theta}_t) = \sigma^2 + \sum_{i=1}^{d} U_i(t)$. We start by considering one such U-shaped curve, and find its minimum as a function of the number of iterations, $t$. Towards this end, we set the derivative of one such U-shaped curve, given by

$$ \frac{\partial}{\partial k} U_i(t) = \sigma_i^2 (\theta_i^*)^2 2 \log(1 - \eta_i \sigma_i^2)(1 - \eta_i \sigma_i^2)^t + \frac{\sigma_i^2}{n} 2((1 - \eta_i \sigma_i^2)^t - 1) \log(1 - \eta_i \sigma_i^2)(1 - \eta_i \sigma_i^2)^t $$

$$ = 2 \log(1 - \eta_i \sigma_i^2)(1 - \eta_i \sigma_i^2)^t \left( (1 - \eta_i \sigma_i^2)^t (\sigma_i^2 (\theta_i^*)^2 + \sigma_i^2/n) - \frac{\sigma_i^2}{n} \right) $$

to zero, which gives that the minimum occurs when

$$ \eta_i = \frac{1}{\sigma_i^2} \left( 1 - \left( \frac{\sigma_i^2/n}{\sigma_i^2 (\theta_i^*)^2 + \sigma_i^2/n} \right)^{1/t} \right). $$

For the iteration $t$ which satisfies this equation, we get

$$ \min_t U_i(t) = \frac{\sigma_i^2/n \sigma_i^2 (\theta_i^*)^2}{\sigma_i^2/n + \sigma_i^2 (\theta_i^*)^2}, $$

thus this minimum is independent of the iteration $t$ and independent of the stepsize, provided their relation is as described in (17) above.
### D Proof and statements for neural networks

In this section, we prove the following result, which is a slightly more formal version of our main result for neural networks, Theorem 2.

**Theorem 3.** Draw a dataset \( \mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\} \) consisting of \( n \) examples i.i.d. from a distribution with \( \|x_i\|_2 = 1 \) and \( |y_i| \leq 1 \). Let \( \Sigma \in \mathbb{R}^{n \times n} \) be the corresponding Gram matrix defined in (7), and suppose its smallest singular value obeys \( \alpha > 0 \).

Pick an error parameter \( \xi \in (0, 1) \) and a failure probability \( \delta \in (0, 1) \), and consider the two-layer neural network \( f_{W, v}(x) = \frac{1}{\sqrt{k}} \text{relu}(x^T W)v \), with parameters \( W^{d \times k}, v \in \mathbb{R}^k \) initialized according to (6) with initialization scale parameters \( \nu, \omega \) obeying \( \nu \omega \leq \frac{\xi}{\sqrt{32 \log(2n/\delta)}} \) and \( \nu + \omega \leq 1 \). Suppose that the network is sufficiently overparameterized, i.e.,

\[
    k \geq \Omega \left( \frac{n^{10}}{\alpha^{11} \min(\nu, \omega) \xi^4} \right). \tag{18}
\]

Then, the risk of the network trained with gradient descent with constant stepsize \( \eta \) for \( t \) iterations obeys, with probability at least \( 1 - \delta \),

\[
    R(f_{W_t, v_t}) \leq \sqrt{\frac{1}{n} \sum_{i=1}^{n} \langle u_i, y \rangle^2 (1 - \eta \sigma_i^2)^{2t}} + \sqrt{\frac{1}{n} \sum_{i=1}^{n} \langle u_i, y \rangle^2 \frac{1 - (1 - \eta \sigma_i^2)^{2t}}{\sigma_i^2}} + \frac{1}{\sqrt{n}} + O(\xi/\alpha). \tag{19}
\]

Theorem 2 directly follows by choosing the error parameter as \( \xi = O(\alpha) \).

#### D.1 Proof of Theorem 3

In this section, we provide a proof of Theorem 2. Our proof relies on the observation that highly overparameterized neural networks behave as associated linear models, as established in a large number of prior works [Aro+19; Du+18; OS20; Oym+19; HS20b].

The proof consists of two parts. First, we control the empirical risk as a function of the number of gradient descent steps, \( t \). Second, we control the generalization error, i.e., the gap between the population risk and the empirical risk by bounding the Rademacher complexity of the function class consisting of two-layer networks trained with \( t \) iterations of gradient descent. Recall that our result depends on the singular values and vectors of the Gram matrix of kernels associated with the two-layer network. The Gram matrix is given as the expectation of the outer product of the Jacobian of the network at initialization:

\[
    \Sigma = \mathbb{E} \left[ \mathcal{J}(W_0, v_0)\mathcal{J}^T(W_0, v_0) \right] = \sum_{i=1}^{n} \sigma_i^2 u_i u_i^T.
\]

Here, expectation is with respect to the random initialization \( W_0, v_0 \).

**Bound on the training error:** We start with a results that controls the training error and ensures that the coefficients of the neural network move little from its initialization.
Theorem 4. Pick an error parameter $\xi \in (0, 1)$ and any failure probability $\delta \in (0, 1)$, and choose $\nu, \omega$ so that they satisfy $\nu \omega \leq \xi / \sqrt{32 \log(2n/\delta)}$. Suppose that the network is sufficiently overparameterized, i.e.,

$$k \geq \Omega \left( \frac{n^{10}(\nu + \omega)^9}{\alpha^{11} \min(\nu, \omega)^{\xi^4}} \right).$$  \hfill (20)

i) Then, with probability at least $1 - \delta$, the mean squared loss after $t$ iterations of gradient descent obeys

$$\sqrt{\sum_{i=1}^{n} (y_i - f_{W_t, v_t}(x_i))^2} \leq \sqrt{\sum_{i=1}^{n} (1 - \eta \sigma_i^2)^{2t} \langle u_i, y \rangle^2 + \xi \|y\|_2^2}.  \hfill (21)$$

ii) Moreover, the coefficients overall deviate little from its initialization, i.e.,

$$\sqrt{\|W_t - W_0\|_F^2 + \|v_t - v_0\|_2^2} \leq \sqrt{\sum_{i=1}^{n} \left( \frac{\langle u_i, y \rangle}{\sigma_i} \left( \frac{1 - (1 - \eta \sigma_i^2)^{2t}}{\sigma_i} \right)^2 \right) + \frac{\xi}{\alpha} \sqrt{n}}. \hfill (22)$$

Here, $\|\cdot\|_F$ denotes the Frobenius norm. In addition each of the coefficients changes only little, i.e., for all iterations $t$

$$\|w_{t, r} - w_{0, r}\|_2 \leq (\nu + \frac{4}{\alpha} \sqrt{n}) \frac{n}{\sqrt{k} \alpha^2}, \hfill (23)$$

$$|v_{t, r} - v_{0, r}| \leq \left( O(\omega \sqrt{\log(nk/\delta)}) + \frac{4}{\alpha} \sqrt{n} \right) \frac{n}{\sqrt{k} \alpha^2}. \hfill (24)$$

Here, $w_{t, r}$ is the $r$-th row of $W_t$, and $v_{t, r}$ is the $r$-th entry of $v_t$.

Bound on the empirical risk: Because we train with respect to the $\ell_2$-loss but define the risk with respect to the (generic Lipschitz) loss $\ell$, the empirical risk and training loss are not the same. Nevertheless, we can upper bound the empirical risk computed over the training set at iteration $t$ with the training loss at iteration $t$:

$$\hat{R}(f_{W_t, v_t}) = \frac{1}{n} \sum_{i=1}^{n} \ell(f_{W_t, v_t}(x_i), y_i)$$

$$\leq \frac{1}{n} \sum_{i=1}^{n} |f_{W_t, v_t}(x_i) - y_i|$$

$$\leq \sqrt{\frac{1}{n} \sum_{i=1}^{n} (f_{W_t, v_t}(x_i) - y_i)^2}$$

$$\leq \sqrt{\frac{1}{n} \sum_{i=1}^{n} \langle u_i, y \rangle^2 (1 - \eta \sigma_i^2)^{2t} + \xi},$$
where (i) follows from \( \ell(z, y) = \ell(z, y) - \ell(y, y) \leq |z - y| \) because the loss is 1-Lipschitz. Equation (ii) is the most interesting one, and follows from Theorem 4, equation (21), and holds with probability at least \( 1 - \delta \). This bound is proven by showing that, provided the network is sufficiently wide, the training loss behaves as gradient descent applied to a linear least-squares problem with dynamics governed by the gram matrix \( \Sigma \).

**Bound on the generalization error:** Next, we bound the generalization error \( R(f) - \hat{R}(f) \) by bounding the Rademacher complexity of the functions that gradient descent can reach with \( t \) gradient descent iterations.

Let \( \mathcal{F} \) be a class of functions \( f: \mathbb{R}^d \rightarrow \mathbb{R} \). Let \( \epsilon_1, \ldots, \epsilon_n \) be iid Rademacher random variables, i.e., random variables that are chosen uniformly from \( \{-1, 1\} \). Given the dataset \( D \), define the empirical Rademacher complexity of the function class \( \mathcal{F} \) as

\[
\mathcal{R}_D(\mathcal{F}) = \frac{1}{n} \mathbb{E}_e \left[ \sup_{f \in \mathcal{F}} \sum_{i=1}^n \epsilon_i f(x_i) \right].
\]

Here, \( D = \{(x_1, y_1), \ldots, (x_n, y_n)\} \) is the training set, consisting of \( n \) points drawn iid from the example generating distribution. By a standard result from statistical learning theory, a bound on the Rademacher complexity directly gives a bound on the generalization error for each predictor in a class of predictors.

**Theorem 5** ([Moh+12, Thm. 3.1]). Suppose \( \ell(\cdot, \cdot) \) is bounded in \([0, 1]\) and 1-Lipschitz in its first argument. With probability at least \( 1 - \delta \) over the random dataset \( D \) consisting of \( n \) iid examples, we have that

\[
\sup_{f \in \mathcal{F}} R(f) - \hat{R}(f) \leq 2\mathcal{R}_D(\mathcal{F}) + 3 \sqrt{\frac{\log(2/\delta)}{2n}}.
\]

We consider the class of neural networks with weights close to the random initialization \( W_0, v_0 \), defined as:

\[
\mathcal{F}_{Q,M} = \{ f_{W,v} : W \in \mathcal{W}, v \in \mathcal{V} \},
\]

with

\[
\mathcal{W} = \{ W : \|W - W_0\|_F \leq Q, \|w_r - w_{0,r}\|_2 \leq \omega M, \text{ for all } r \},
\]

\[
\mathcal{V} = \{ v : \|v - v_0\|_2 \leq Q, \|v_r - v_{0,r}\| \leq \nu M, \text{ for all } r \}.
\]

The Rademacher complexity of this class of functions is controlled with the following result.

**Lemma 4.** Let \( W_0 \) be drawn from a Gaussian distribution with \( \mathcal{N}(0, \omega^2) \) entries, and suppose the entries of \( v_0 \) are drawn uniformly from \( \{-\nu, \nu\} \). Assume the \( (x_i, y_i) \) are drawn iid from some distribution with \( \|x_i\|_2 = 1 \) and \( |y_i| \leq 1 \). With probability at least \( 1 - \delta \) over the random training set, provided that \( \sqrt{\log(2n/\delta)/2k} \leq 1/2 \), the empirical Rademacher complexity of \( \mathcal{F}_{Q,M} \) is, simultaneously for all \( Q \), bounded by

\[
\mathcal{R}_D(\mathcal{F}_{Q,M}) \leq \frac{Q}{\sqrt{n}} (\nu + \omega) + \nu \omega (5M^2 \sqrt{k} + 4M \sqrt{\log(2/\delta)/2}).
\]
We set \( M = O(\xi^{1/4}) \). With this choice, the term on the right hand side above is bounded by
\[
\nu \omega (5M^2 \sqrt{k} + 4M \sqrt{\log(2/\delta)/2}) \leq O(\xi/\alpha),
\]
where we used \( \nu \omega \leq 1 \) and \( \sqrt{\log(2/\delta)/2} \leq 1 \), by assumption (18). Note that by (23) and by (24) combined with the assumption (18) we have that \( \|w_r - w_{0,r}\|_2 \leq \omega M \) and \( |v_r - v_{0,r}| \leq \nu M \), as desired.

Let \( Q_i = i \) for \( i = 1, 2, \ldots \). Simultaneously for all \( i \), by the lemma above, for this choice of \( M \), the function class \( \mathcal{F}_{Q_i,M} \) has Rademacher complexity bounded by
\[
\mathcal{R}_D(\mathcal{F}_{Q_i,M}) \leq \frac{Q_i}{\sqrt{n}} (\nu + \omega) + O(\xi/\alpha).
\]
(27)

We next choose the radius \( Q \) as defined in (22). Let \( i^* \) be the smallest integer such that \( Q \leq Q_{i^*} \), so that \( Q_{i^*} \leq Q + 1 \). We have that \( i^* \leq O(\sqrt{n}/\alpha) \) and
\[
\mathcal{R}_D(\mathcal{F}_{Q_{i^*},M}) \leq \frac{(Q + 1)}{\sqrt{n}} (\nu + \omega) + O(\xi/\alpha)
\]
\[
\leq \frac{1}{n} \sum_{i=1}^{n} \left( \langle u_i, y \rangle \frac{1 - (1 - \eta \sigma^2_i)^t}{\sigma_i} \right)^2 + \frac{1}{\sqrt{n}} + O(\xi/\alpha),
\]
(28)

by the assumption of the theorem on \( k \) being sufficiently large, and by \( \nu + \omega \leq 1 \). Next, from a union bound over the finite set of integers \( i = 1, \ldots, i^* \), we obtain
\[
\max_{i=1,\ldots,i^*} \sup_{f \in \mathcal{F}_{Q_i,M}} R(f) - \hat{R}(f) \leq \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left( \langle u_i, y \rangle \frac{1 - (1 - \eta \sigma^2_i)^t}{\sigma_i} \right)^2 + \frac{1}{\sqrt{n}} + O(\xi/\alpha)},
\]
(29)
as desired.

**Final bound on the risk:** Combining the bound on the training with the generalization bound yields the upper bound (19) on the risk of the network trained for \( t \) iterations of gradient descent.

The remainder of the proof is devoted to proving Theorem 4 and Lemma 4.

### D.2 Preliminaries

We start with introducing some useful notation. First note that the prediction of the neural network for the \( n \) training data points as a function of the parameters are
\[
f(W, v) = \frac{1}{\sqrt{k}} \begin{bmatrix} \text{relu}(x_1^T W) v \\ \vdots \\ \text{relu}(x_n^T W) v \end{bmatrix} = \frac{1}{\sqrt{k}} \text{relu}(XW)v,
\]
(30)

where \( X^{n \times d} \) is the feature matrix and \( W \in \mathbb{R}^{d \times k} \) and \( v \in \mathbb{R}^k \) are the trainable weights of the network. The transposed Jacobian of the function \( f \) is given by
\[
J^T(W, v) = \begin{bmatrix} J_1^T(W, v) \\ J_2^T(W) \end{bmatrix} \in \mathbb{R}^{dk+k \times n},
\]
(31)
where we defined the Jacobians corresponding to the weights of the first layer, $W$, and the second layer, $v$, respectively as

$$J_T^1(W, v) = \frac{1}{\sqrt{k}} \begin{bmatrix} v_1 X^T \text{diag}(\text{relu}'(Xw_1)) \\ \vdots \\ v_t X^T \text{diag}(\text{relu}'(Xw_t)) \end{bmatrix} \in \mathbb{R}^{dk \times n}, \quad J_T^2(W) = \frac{1}{\sqrt{k}} \text{relu}(XW)^T \in \mathbb{R}^{k \times n}.$$ 

Here, $\text{relu}'(x) = 1_{\{x \geq 0\}}$ is the derivative of the relu activation function, which is the step function. Our results depend on the singular values and vectors of the expected Jacobian at initialization:

$$\mathbb{E} \left[ J(W_0, v_0) J^T(W_0, v_0) \right] = \nu^2 \sum_{\ell=1}^{k} \mathbb{E} \left[ \text{relu}'(Xw_\ell) \text{relu}'(Xw_\ell)^T \right] \odot XX^T$$

$$+ \frac{1}{k} \mathbb{E} \left[ \text{relu}(XW_0) \text{relu}(XW_0)^T \right],$$

where $\odot$ is the Hadamard product, and where we used that the entries of $v_0$ are chosen iid uniformly from $\{-\nu, \nu\}$. Expectation is over the weights $W_0$ at initialization, which are iid $\mathcal{N}(0, \omega^2)$. This yields

$$[\mathbb{E} \left[ J(W_0, v_0) J^T(W_0, v_0) \right]]_{ij} = \nu^2 K_1(x_i, x_j) + \omega^2 K_2(x_i, x_j), \quad (32)$$

where $K_1$ and $K_2$ are two kernels associated with the first and second layers of the network and are given by

$$K_1(x_i, x_j) = \left[ \mathbb{E} \left[ \text{relu}'(Xw_\ell) \text{relu}'(Xw_\ell)^T \right] \right]_{ij}$$

$$= \frac{1}{2} \left( 1 - \cos^{-1}(\rho_{ij}) / \pi \right) \langle x_i, x_j \rangle$$

with $\rho_{ij} = \langle x_i, x_j \rangle / \|x_i\|_2 \|x_j\|_2$ and by

$$K_2(x_i, x_j) = \frac{1}{\omega^2 k} \mathbb{E} \left[ \text{relu}(XW) \text{relu}(XW)^T \right]_{ij}$$

$$= \frac{1}{\omega^2} \left[ \mathbb{E} \left[ \text{relu}(Xw) \text{relu}(Xw)^T \right] \right]_{ij}$$

$$= \frac{1}{2} \left( \sqrt{1 - \rho_{ij}^2 / \pi} + (1 - \cos^{-1}(\rho_{ij}) / \pi) \rho_{ij} \right) \|x_i\|_2 \|x_j\|_2.$$ 

For both of those expressions, we used the calculations from [Dan+16, Sec. 4.2] for the final expressions of the kernels. Also note that, by assumption $\|x_i\|_2 = 1$.

### D.3 Proof of Theorem 4 (bound on the training error)

In this subsection, we prove Theorem 4.
D.3.1 The dynamics of linear and nonlinear least-squares

Theorem 4 relies on approximating the trajectory of gradient descent applied to the training loss with an associated linear model that approximates the non-linear neural network in the highly-overparameterized regime. This strategy has been used in a number of recent publications [Aro+19; Du+18; OS20; Oym+19; HS20b]; in order to avoid repetition, we rely on a statement [HS20a, Theorem 4], which bounds the error between the true trajectory of gradient descent and the trajectory of an associated linear problem.

Let \( f: \mathbb{R}^N \to \mathbb{R}^n \) be a non-linear function with parameters \( \theta \in \mathbb{R}^N \), and consider the non-linear least squares problem

\[
L(\theta) = \frac{1}{2} \| f(\theta) - y \|_2^2.
\]

The gradient descent iterations starting from an initial point \( \theta_0 \) are given by

\[
\theta_{t+1} = \theta_t - \eta \nabla L(\theta_t) \quad \text{where} \quad \nabla L(\theta) = J^T(\theta)(f(\theta) - y),
\]

where \( J(\theta) \in \mathbb{R}^{n \times N} \) is the Jacobian of \( f \) at \( \theta \) (i.e., \( [J(\theta)]_{i,j} = \frac{\partial f_i(\theta)}{\partial \theta_j} \)). The associated linearized least-squares problem is defined as

\[
L_{\text{lin}}(\theta) = \frac{1}{2} \| f(\theta_0) + J(\theta - \theta_0) - y \|_2^2.
\]

Here, \( J \in \mathbb{R}^{n \times N} \), referred to as the reference Jacobian, is a fixed matrix independent of the parameter \( \theta \) that approximates the Jacobian mapping at initialization, \( J(\theta_0) \). Starting from the same initial point \( \theta_0 \), the gradient descent updates of the linearized problem are

\[
\hat{\theta}_{t+1} = \hat{\theta}_t - \eta J^T \left( f(\theta_0) + J(\hat{\theta}_t - \theta_0) - y \right).
\]

To show that the non-linear updates (33) are close to the linearized iterates (35), we make the following assumptions:

i) We assume that the singular values of the reference Jacobian obey for some \( \alpha, \beta \)

\[
\sqrt{2} \alpha \leq \sigma_n \leq \sigma_1 \leq \beta.
\]

Furthermore, we assume that the norm of the Jacobian associated with the nonlinear model \( f \) is bounded in a radius \( R \) around the random initialization

\[
\| J(\theta) \| \leq \beta \quad \text{for all} \quad \theta \in B_R(\theta_0).
\]

Here, \( B_R(\theta_0) := \{ \theta : \| \theta - \theta_0 \| \leq R \} \) is the ball with radius \( R \) around \( \theta_0 \).

ii) We assume the reference Jacobian and the Jacobian of the nonlinearity at initialization \( J(\theta_0) \) are \( \epsilon_0 \)-close:

\[
\| J(\theta_0) - J \| \leq \epsilon_0.
\]

iii) We assume that within a radius \( R \) around the initialization, the Jacobian varies by no more than \( \epsilon \):

\[
\| J(\theta) - J(\theta_0) \| \leq \frac{\epsilon}{2} \quad \text{for all} \quad \theta \in B_R(\theta_0).
\]
Under these assumptions the difference between the non-linear residual
\[ r_t := f(\theta_t) - y \]
and the linear residual
\[ \tilde{r}_t := f(\theta_0) + J(\tilde{\theta}_t - \theta_0) - y \]
are close throughout the entire run of gradient descent.

**Theorem 6** ([HS20a, Theorem 4], Closeness of linear and nonlinear least-squares problems). Assume the Jacobian \( J(\theta) \in \mathbb{R}^{n \times N} \) associated with the function \( f(\theta) \) obeys Assumptions (36a), (36b), (36c), and (36d) around an initial point \( \theta_0 \in \mathbb{R}^N \) with respect to a reference Jacobian \( J \in \mathbb{R}^{n \times N} \) and with parameters \( \alpha, \beta, \epsilon_0, \epsilon \), obeying \( 2\beta(\epsilon_0 + \epsilon) \leq \alpha^2 \), and \( R \). Furthermore, assume the radius \( R \) is given by

\[
R := 2\left\| J^\dagger r_0 \right\|_2^2 + \frac{\beta^2}{\alpha^4}(\epsilon_0 + \epsilon)\|r_0\|_2^2.
\]

(37)

Here, \( J^\dagger \) is the pseudo-inverse of \( J \). We run gradient descent with stepsize \( \eta \leq \frac{1}{\beta^2} \) on the linear and non-linear least squares problem, starting from the same initialization \( \theta_0 \). Then, for all iterations \( t \),

i) the non-linear residual converges geometrically

\[
\|r_t\|_2 \leq (1 - \eta \alpha^2)^t \|r_0\|_2,
\]

(38)

ii) the residuals of the original and the linearized problems are close

\[
\|r_t - \tilde{r}_t\|_2 \leq \frac{2\beta(\epsilon_0 + \epsilon)}{\epsilon(\ln 2)\alpha^2}\|r_0\|_2.
\]

(39)

iii) the parameters of the original and the linearized problems are close

\[
\|\theta_t - \tilde{\theta}_t\|_2 \leq 2.5\frac{\beta^2}{\alpha^4}(\epsilon_0 + \epsilon)\|r_0\|_2,
\]

(40)

iv) and the parameters are not far from the initialization

\[
\|\theta_t - \theta_0\|_2 \leq \frac{R}{2}.
\]

(41)

Theorem 6 above formalizes that in a (small) radius around the initialization, the non-linear problem behaves very similar to its associated linear problem. As a consequence, to characterize the dynamics of the nonlinear problem, it suffices to characterize the dynamics of the linearized problem. This is the subject of our next theorem, which is a standard result on the gradient iterations of a least squares problem, see for example [HS20b, Thm. 5] for the proof.

25
Theorem 7 (E.g. Theorem 5 in [HS20b]). Consider a linear least squares problem \((34)\) and let \(J = \sum_{i=1}^{n} \sigma_i u_i v_i^T\) be the singular value decomposition of the matrix \(J\). Then the linear residual \(\tilde{r}_t\) after \(t\) iterations of gradient descent with updates \((35)\) is
\[
\tilde{r}_t = \sum_{i=1}^{n} \left(1 - \eta \sigma_i^2\right)^t u_i \langle u_i, r_0 \rangle .
\]
Moreover, using a step size satisfying \(\eta \leq \frac{1}{\sigma_i^2}\), the linearized iterates \((35)\) obey
\[
\|\hat{\theta}_t - \theta_0\|^2 = \sum_{i=1}^{n} \left|\langle u_i, r_0 \rangle \left(1 - \frac{(1 - \eta \sigma_i^2)^t}{\sigma_i^2}\right)\right|^2 .
\]

D.3.2 Proving Theorem 4 by applying Theorem 6

We are now ready to prove Theorem 4. We apply Theorem 6 to the predictions of the network given by \(f(W,v)\) defined in \((30)\) with parameter \(\theta = (W,v)\). As reference Jacobian we choose a matrix \(J \in \mathbb{R}^{n \times dk+k}\) that satisfies \(JJ^T = \mathbb{E} [J(W_0,v_0)J^T(W_0,v_0)]\) (where expectation is over the random initialization \((W_0,v_0)\)), and at the same time is very close to the Jacobian of \(f\) at initialization, i.e., to \(J(W_0,v_0)\). Towards this goal, we apply Theorem 6 with the following choices of parameters:
\[
\alpha = \sigma_{\min}(\Sigma)/\sqrt{2}, \quad \beta = 10 \sqrt{n}(\omega + \nu), \quad \epsilon = \frac{1}{16} \frac{\epsilon^3}{\beta^2}, \quad \epsilon_0 = 2 \sqrt{(\omega^2 + \nu^2) \frac{3n}{\sqrt{k}} \log(kn/\delta)} .
\]
Note that assumption \((20)\) guarantees that \(\epsilon_0 \leq \epsilon\), a fact we used later.

We now verify that the conditions of Theorem 4 are satisfied for this choice of parameters with probability at least \(1 - \delta\). Specifically we show that each of the conditions holds with probability at least \(1 - \delta\). By a union bound, the success probability is then at least \(1 - \Omega(\delta)\), and by rescaling \(\delta\) by a constant, the conditions are satisfied with probability at least \(1 - \delta\).

Bound on residual: We need a bound on the network outputs at initialization as well as on the initial residual to verify the conditions of the theorem. We start with the former:
\[
\|f(W_0,v_0)\|_2 = \frac{1}{\sqrt{k}} \|\text{relu}(XW_0)v_0\|_2 \leq \nu \omega \sqrt{8 \log(2n/\delta)} \|X\|_F = \nu \omega \sqrt{8 \log(2n/\delta)} \sqrt{n} ,
\]
where the inequality holds with probability at least \(1 - \delta\), by Gaussian concentration (see Lemma 6 in [HS20b] and recall that \(W_0\) has iid \(N(0,\omega^2)\) entries). Moreover, the last equality follows from \(\|x_i\|_2 = 1\).

It follows that, with probability at least \(1 - \delta\), the initial residual is bounded by
\[
\|r_0\|_2 = \left\|\frac{1}{\sqrt{k}} \text{relu}(XW_0)v_0 - y\right\|_2 \leq \nu \omega \sqrt{8 \log(2n/\delta)} \sqrt{n} + \sqrt{n} \leq 2\sqrt{n} .
\]
where the first inequality holds by the triangle inequality and using the assumption $|y_i| \leq 1$, and the second inequality by $\nu \omega \sqrt{8 \log(2n/\delta)} \leq 1$, again by assumption.

**Radius in the theorem:** In order to verify the condition of the theorem, we need to control the radius in the theorem, which we do next. With our assumptions and the choices of parameters above, the radius in the theorem, defined in equation (37), obeys

$$R = 2\left\| J^* r_0 \right\|_2 + 5 \beta^2 \alpha^4 (\epsilon_0 + \epsilon) \left\| r_0 \right\|_2$$

(i) $$\leq \left( \frac{\sqrt{2}}{\alpha} + 5 \frac{\beta^2}{\alpha^4} (\epsilon_0 + \epsilon) \right) \left\| r_0 \right\|_2$$

(ii) $$\leq \left( \frac{\sqrt{2}}{\alpha} + \frac{5}{16} \alpha \right) \left\| r_0 \right\|_2$$

(iii) $$\leq \frac{4}{\alpha} \sqrt{n}$$

(iv) $$\leq \min(\omega, \nu) \sqrt{k} \left( \frac{16 \xi \alpha^3 \beta^2}{10 (\nu + 3 \omega)} \right)^3 \tilde{R}.$$

Here, (i) follows from the fact that $\left\| J^* r_0 \right\|_2 \leq \frac{1}{\sqrt{2\alpha}} \left\| r_0 \right\|_2$, (ii) from $\epsilon_0 + \epsilon \leq 2 \epsilon = \frac{1}{8} \xi \alpha^3 \beta^2$ (by definition of $\epsilon_0$ and $\epsilon$), and (iii) from the bound on the residual (46). For (iv) we used assumption (20) in the theorem.

**Verifying Assumptions (36a) and (36b):** By definition $JJ^T = \Sigma$, thus the lower bound in assumption (36a) holds by the definition of $\alpha$ as $\sigma_n(\Sigma) \geq \sqrt{2\alpha}$. Regarding the upper bound of (36a), note that

$$\left\| J \right\|^2 \leq \nu^2 \left\| K_1 \right\|_F + \omega^2 \left\| K_2 \right\|_F$$

$$\leq \nu^2 n + \omega^2 n,$$

where $K_1 \in \mathbb{R}^{n \times n}$ and $K_2 \in \mathbb{R}^{n \times n}$ are the kernel matrix with entries $K_1(x_i, x_j)$ and $K_2(x_i, x_j)$. It follows that $\left\| J \right\| \leq 2(\omega + \nu) \sqrt{n} \leq \beta$, as desired. This concludes the verification of (36a).

To verify assumption (36b) note that

$$\left\| J(W, v) \right\| \leq \left\| J_1(W) \right\| + \left\| J_2(W) \right\|$$

$$\leq \frac{1}{\sqrt{k}} (\left\| X \right\| \left\| v \right\|_2 + \left\| XW \right\|_F)$$

$$\leq \frac{1}{\sqrt{k}} \left( \left\| X \right\| (\left\| v_0 \right\|_2 + \left\| v - v_0 \right\|_2 + \left\| W - W_0 \right\|_F) + \left\| XW_0 \right\|_F \right)$$

$$\leq \sqrt{n} \frac{10(\omega + \nu)}{\sqrt{k}} = \beta.$$

For the last inequality, we used that $\left\| v_0 \right\|_2 = \nu \sqrt{k}$, and that $\left\| v - v_0 \right\|_2 + \left\| W - W_0 \right\|_F \leq R \leq \sqrt{k} \min(\omega, \nu)$, by the bound on the radius in (47), and finally that $\left\| XW_0 \right\|_F \leq \omega \nu \sqrt{k}$ with probability at least $1 - \delta$ provided that $k \geq \log(n/\delta)$, which holds by assumption. For this inequality we
used that $x_T^T W_0$ is a Gaussian vector with iid $N(0, \omega^2)$ entries. It follows that assumption (36b) holds with probability at least $1 - \delta$, as desired.

Verifying Assumption (36c): We start with stating a concentration lemma from [HS20b].

**Lemma 5** (Concentration lemma [HS20b, Lemma 3]). Consider the partial Jacobian $J_1(W)$, and let $W \in \mathbb{R}^{n \times k}$ be generated at random with i.i.d. $N(0, \omega^2)$ entries, and suppose the $v_\ell$ are drawn from a distribution with $|v_\ell| \leq \nu$. Then, with probability at least $1 - \delta$,

$$
\left\| J_1(W, v) J_1^T(W, v) - \mathbb{E} \left[ J_1(W, v) J_1^T(W, v) \right] \right\| \leq \frac{\nu^2}{\sqrt{k}} \|X\|^2 \sqrt{\log (2n/\delta)}.
$$

**Lemma 6.** Let $J_2(W) = \frac{1}{\sqrt{k}} \text{relu}(XW)$, with $W$ generated at random with i.i.d. $N(0, \omega^2)$ entries. With probability at least $1 - \delta$,

$$
\left\| J_2(W) J_2^T(W) - \mathbb{E} \left[ J_2(W) J_2^T(W) \right] \right\| \leq \frac{3 \omega^2}{\sqrt{k}} \|X\|^2 \log (kn/\delta). \tag{48}
$$

Combining the statements of the two lemmas, it follows that, with probability at least $1 - 2\delta$,

$$
\left\| J(W, v) J^T(W, v) - \mathbb{E} \left[ J(W, v) J^T(W, v) \right] \right\| \leq (\omega^2 + \nu^2) \frac{1}{\sqrt{k}} \|X\|^2 \log (kn/\delta)
\leq (\omega^2 + \nu^2) \frac{3}{\sqrt{k}} n \log (kn/\delta). \tag{49}
$$

To show that (49) implies the condition in (36c), we use the following lemma.

**Lemma 7** ([Oym+19, Lem. 6.4]). Let $J_0 \in \mathbb{R}^{n \times N}$, $N \geq n$ and let $\Sigma$ be an $n \times n$ psd matrix obeying $\|J_0 J_0^T - \Sigma\| \leq \tilde{c}^2$, for a scalar $\tilde{c} \geq 0$. Then there exists a matrix $J \in \mathbb{R}^{n \times N}$ obeying $\Sigma = JJ^T$ such that

$$
\|J - J_0\| \leq 2\tilde{c}.
$$

From Lemma 7 combined with equation (49), there exists a matrix $J \in \mathbb{R}^{n \times N}$ that obeys

$$
\|J - J(W_0, v_0)\| \leq \epsilon_0, \quad \epsilon_0 = 2 \sqrt{(\omega^2 + \nu^2) \frac{3n}{\sqrt{k}} \log (kn/\delta)}.
$$

This part of the proof also specifies our choice of the matrix $J$ as a matrix that is close to the Jacobian at initialization, $J(W_0)$, and that exists by Lemma 7 above.

Verifying Assumption (36d): We control the perturbation around the random initialization.

**Lemma 8.** Let $W_0$ have iid $N(0, \omega^2)$ entries and let $v_0$ have (arbitrary) entries in $\{-\nu, +\nu\}$ entries. Then for all $W$ and $v$ obeying, for some $\tilde{R} \leq \frac{3}{2} \sqrt{k}$,

$$
\|W - W_0\|_{F} \leq \omega \tilde{R}, \quad \|v - v_0\|_2 \leq \nu \tilde{R},
$$

the Jacobian in (31) obeys

$$
\|J(W, v) - J(W_0, v_0)\| \leq \|X\| \frac{1}{\sqrt{k}} \left( \omega \tilde{R} + \nu \tilde{R} + \nu \sqrt{2} (2t \tilde{R})^{1/3} \right),
$$

with probability at least $1 - ne^{-\frac{1}{2} \tilde{R}^{3/2} k^{7/3}}$. 

28
Recall the definition \( \tilde{R} = \sqrt{k}\left(\frac{\epsilon}{\|X\| (\nu + 3\omega)}\right)^3 \) from (47). From \( \tilde{R} \leq (kR)^{1/3} \) for \( \tilde{R} \leq \sqrt{k} \), the bound provided by lemma 8 guarantees that

\[
\|J(W, v) - J(W_0, v_0)\| \leq \|X\| \frac{\omega + 3\nu}{\sqrt{k}} (k\tilde{R})^{1/3}
\]

\[
= \epsilon = \frac{1}{16} \frac{\alpha^3}{\beta^2},
\]

where the second inequality follows by choosing \( \tilde{R} = \sqrt{k}\left(\frac{\epsilon}{\|X\| (\nu + 3\omega)}\right)^3 \). This holds with probability at least

\[
1 - ne^{-\frac{1}{2}R^7/3} = 1 - ne^{-2^{-17} \xi^4 \frac{\epsilon^3}{\beta^3}} \geq 1 - \delta,
\]

where in (i) we used (20). Therefore, Assumption (36d) holds with high probability by our choice of \( \epsilon = \frac{1}{16} \frac{\alpha^3}{\beta^2} \).

**Concluding the proof of Theorem 4:** By the previous paragraphs, the assumptions of Theorem 4 are satisfied with probability at least \( 1 - O(\delta) \). Therefore we can bound the training error and the deviation of the coefficients from the initialization as follows.

**Training error:** We bound the training error in (20). The training error at iteration \( t \) is bounded by

\[
\|f(W_t, v_t) - y\|_2 \leq \|\tilde{r}_t\|_2 + \|\tilde{r}_t - r_t\|_2
\]

\[
\leq \left(\sum_{i=1}^n (1 - \eta \sigma_i^2)^{2t} \langle u_i, r_0 \rangle^2\right)^{1/2} + \frac{2\beta (\epsilon_0 + \epsilon)}{e(\ln 2)\alpha^2} \|r_0\|_2
\]

\[
\leq \left(\sum_{i=1}^n (1 - \eta \sigma_i^2)^{2t} \langle u_i, y \rangle^2\right)^{1/2} + \|f(W_0, w_0)\|_2 + \frac{2\beta (\epsilon_0 + \epsilon)}{e(\ln 2)\alpha^2} \|r_0\|_2
\]

\[
\leq \left(\sum_{i=1}^n (1 - \eta \sigma_i^2)^{2t} \langle u_i, y \rangle^2\right)^{1/2} + \xi \|y\|_2
\]

where inequality (i) follows from bounding the linear residual \( \|\tilde{r}_t\|_2 \) with theorem 7, as well as bounding the distance between the linear residual and the non-linear one with (39). Inequality (ii) follows from \( r_0 = f(W_0, v_0) - y \), and finally (iii) follows from \( \|f(W_0, v_0)\|_2 \leq \nu \omega \sqrt{8 \log(2n/\delta)} \|y\|_2 \leq \frac{\xi}{2} \|y\|_2 \), by (45), and \( \frac{\beta}{\alpha^2}(\epsilon_0 + \epsilon) \leq \frac{\beta}{\alpha^2} 2\epsilon = \frac{1}{8} \xi \frac{\alpha^3}{\beta^2} \leq \xi \).
Distance from initialization: We next bound the distance from the initialization, i.e., we establish (22). Combining equation (43) in theorem 7 with equation (39) in theorem 6, we obtain

$$\sqrt{\|W_t - W_0\|_F^2 + \|v_t - v_0\|_2^2} \leq \sum_{i=1}^{n} \left( \frac{1 - (1 - \eta \sigma_i^2)^t}{\sigma_i} \right)^2 + 2.5 \frac{\beta^2}{\alpha^4} (\epsilon_0 + \epsilon) \|r_0\|_2$$

$$\leq \sum_{i=1}^{n} \left( \frac{1 - (1 - \eta \sigma_i^2)^t}{\sigma_i} \right)^2 + \frac{1}{\alpha} \|f(W_0, v_0)\|_2 + 2.5 \frac{\beta^2}{\alpha^4} (\epsilon_0 + \epsilon) \|r_0\|_2$$

Bound on change of coefficients: Finally, we establish the bounds on the change of the individual coefficients (23) and (24). We start with the weights in the first layer, \(w_r\). The gradient with respect to \(w_r\) is given by \(\nabla_{w_r} \mathcal{L}(W, v) = [J^T_1(W, v)]_r, \) where \([J^T_1(W, v)]_r\) is the submatrix of the Jacobian multiplying with the weight \(w_r\), and \(r\) is the residual. Therefore, we obtain

$$\|w_{t,r} - w_{0,r}\|_2^2 = \left\| \sum_{\tau=0}^{t-1} (w_{\tau+1,r} - w_{\tau,r}) \right\|_2^2 \leq \sum_{\tau=0}^{t-1} \eta \|[J^T_1(W_{\tau}, v_{\tau})]_r r_{\tau}\|_2^2$$

$$\leq (\nu + \frac{4}{\alpha} \sqrt{n}) \frac{\sqrt{n}}{\sqrt{k}} \eta \sum_{\tau=0}^{t-1} \|r_{\tau}\|_2$$

Here, (i) follows from

$$\|[J^T_1(W_{\tau}, v_{\tau})]_r\| = \left\| \frac{v_r}{\sqrt{k}} \text{diag} (\text{relu}'(Xw_r)) X \right\| \leq v_r \frac{\sqrt{n}}{\sqrt{k}} \leq (\nu + \frac{4}{\alpha} \sqrt{n}) \frac{\sqrt{n}}{\sqrt{k}}.$$
where the last inequality follows from $|v_{\tau,r} - v_{0,r}| \leq \|v_{\tau,r} - v_{0,r}\|_2 \leq R \leq \frac{1}{\alpha} \sqrt{n}$, by (47). Moreover, for (ii) we used that, by (38), the non-linear residuals converge geometrically, and (iii) follows from the formula for a geometric series. This conclude the proof of the bound (23).

Analogously, we obtain

$$|v_{\tau,r} - v_{0,r}| \leq \sum_{\tau=0}^{t-1} \eta ||J_2^T(W_{\tau})r_{\tau}|| \leq \left(O(\omega \sqrt{\log(nk/\delta)}) + \frac{4}{\alpha} \sqrt{n}\right) \sqrt{n} \frac{1}{\sqrt{k}} \alpha^2 \|r_0\|_2$$

where we used that

$$\frac{1}{\sqrt{k}} \|\text{relu}(Xw) - \text{relu}(Xw')\|_2 \leq \frac{1}{\sqrt{k}} \left(||Xw_0,r||_2 + ||X(w_0,r - w_{r})||_2\right) \leq \frac{1}{\sqrt{k}} \left(O(\omega \sqrt{n \log(nk/\delta)}) + \sqrt{n} ||w_0,r - w_{r}||_2\right) \leq \frac{1}{\sqrt{k}} \left(O(\omega \sqrt{n \log(nk/\delta)}) + \sqrt{n} \frac{4}{\alpha^2}\right).$$

Here, the last inequality follows by using that the entries of $Xw_0,r$ are not independent but $\mathcal{N}(0, \omega^2)$ distributed, and by taking an union bound over all entries of that vector and over all $Xw_{0,r}$. This concludes the proof of the bound (24).

### D.3.3 Proof of lemma 8

First note that

$$\|J(W, v) - J(W', v')\| \leq \|J_1(W, v) - J_1(W', v')\| + \|J_2(W, v) - J_2(W', v')\|$$

$$\leq \|J_1(W, v) - J_1(W', v')\| + \|J_1(W, v') - J_1(W', v')\| + \|J_2(W, v) - J_2(W', v')\|. \quad (50)$$

In the reminder of the proof we bound the three terms above. We start by bounding the third term in (50) as:

$$\|J_2(W, v) - J_2(W', v')\| \leq \frac{1}{\sqrt{k}} \|\text{relu}(XW) - \text{relu}(XW')\|_F \leq \frac{1}{\sqrt{k}} \|XW - XW'\|_F \leq \frac{1}{\sqrt{k}} \|X\| \|W - W'\|_F.$$

31
We proceed with bounding the first term in (50) as:

\[
\|J_1(W, v) - J_1(W, v')\|^2 = \left\| (J_1(W, v) - J_1(W, v'))(J_1(W, v) - J_1(W, v'))^T \right\|
\]

\[
= \frac{1}{k} \| \text{relu}'(XW)\text{diag}((v_1 - v'_1)^2, \ldots, (v_t - v'_t)^2)\text{relu}'(XW)^T \circ XX^T \|
\]

\[
\leq \frac{1}{k} \| X \|^2 \max_j \| \text{relu}'(x^j W)\text{diag}(v - v') \|^2
\]

\[
\leq \frac{1}{k} \| v - v' \|^2 \| X \|^2.
\]

Next we establish below that with probability at least \(1 - ne^{-kq^2/2}\), the second term in in (50) is bounded as

\[
\| J_1(W, v) - J_1(W', v') \| \leq \frac{1}{\sqrt{k}} \| v' \|_\infty \| X \| \sqrt{2q}
\] (51)

provided that

\[
\| W - W' \| \leq \sqrt{\frac{q}{2k}} \omega = \omega \tilde{R},
\]

where the last inequality follows from setting \(q = (2k \tilde{R})^{2/3}\) (note that the assumption \(\tilde{R} \leq \frac{1}{2} \sqrt{k}\) ensures \(q \leq k\)). Putting those three bounds together in (50) yields

\[
\| J(W, v) - J(W', v') \| \leq \| X \| \frac{1}{\sqrt{k}} \left( \| W - W' \|_F + \| v - v' \|_2 + \| v' \|_\infty \sqrt{2(2k \tilde{R})^{1/3}} \right),
\] (52)

which established the claim.

It remains to prove (51). Towards this goal, first note that

\[
\| J_1(W, v) - J_1(W', v') \| \leq \| J_1(W, v) - J_1(W, v') \| + \| J_1(W, v') - J_1(W', v') \|.
\] (53)

We proceed with bounding the second term in the RHS of (53) as:

\[
\| J_1(W, v') - J_1(W', v') \|^2 \leq \frac{1}{k} \| v' \|_\infty^2 \| X \|^2 \max_j \| \sigma'(x^j_iW) - \sigma'(x^j_iW') \|^2.
\] (54)

Because \(\text{relu}'\) is the step function, we have to bound the number of sign flips between the matrices \(XW\) and \(XW'\). For this we use the lemma below:

**Lemma 9.** Let \(v_{\pi(q)}\) be the \(q\)-th smallest entry of \(v\) in absolute value. Suppose that, for all \(i\), and \(q \leq k\),

\[
\| W - W' \| \leq \sqrt{q} \frac{|x^i_iW'|_{\pi(q)}}{\| x^i \|}.
\]

Then

\[
\max_i \| \sigma'(x^i_iW) - \sigma'(x^i_iW') \| \leq \sqrt{2q}.
\]

For the entries \(W'\) being iid \(\mathcal{N}(0, \omega^2)\), we note that, with probability at least \(1 - ne^{-kq^2/2}\), the \(q\)-th smallest entry of \(x^j_iW' \in \mathbb{R}^k\) obeys

\[
\frac{|x^i_iW'|_{\pi(q)}}{\| x^i \|} \geq \frac{q}{2k} \omega \quad \text{for all } i = 1, \ldots, n.
\] (55)
We are now ready to conclude the proof of the lemma. By equation (54),
\[
\| \mathcal{J}_1(W, v') - \mathcal{J}_1(W', v') \| \leq \frac{1}{\sqrt{k}} \| v' \|_{\infty} \| X \| \max_j \| \sigma'(x_j^T W) - \sigma'(x_j^T W') \| \\
\leq \frac{1}{\sqrt{k}} \| v' \|_{\infty} \| X \| \sqrt{2q}
\]
provided that
\[
\| W - W' \| \leq \sqrt{\frac{q}{2k}} \omega
\]
with probability at least 1 - ne^{-kq^2/2}.

## D.4 Proof of Lemma 4 (bound on the Rademacher complexity)

Our proof follows that of a related result, specifically [Aro+19, Lem. 6.4] which pertains to a two-layer ReLU network where only the first layer is trained and the second layers’ coefficients are fixed. Our goal is to bound the empirical Rademacher complexity

\[
\mathcal{R}_D(\mathcal{F}_{Q,M}) = \frac{1}{n} \mathbb{E} \left[ \sup_{W_0, v \in \mathcal{V}} \sum_{i=1}^{n} \epsilon_i \frac{1}{\sqrt{k}} \sum_{r=1}^{k} v_r \text{relu}(w_r^T x_i) \right],
\]

where expectation is over the iid Rademacher random variables \( \epsilon_i \), and where \( \{x_1, \ldots, x_n\} \) are the training examples.

The derivation of the bound on the Rademacher complexity is based on the intuition that if the parameter \( M \) of the constraint \( \| w_r - w_{0,r} \|_2 \leq \omega M \) is sufficiently small, then relu\((w_r^T x_i)\) is constant for most \( r \), because \( |w_r^T x_i| \) is bounded away from \( \omega M \) with high probability, by anti-concentration of a Gaussian. For those coefficient vectors \( r \) for which relu\((w_r^T x_i)\) is constant, we have relu\((w_r^T x_i)\) = relu\((w_{0,r}^T x_i)\)w_r^T x_i. For the other coefficients, we can bound the difference of those two values as

\[
\text{relu}(w_r^T x_i) - \text{relu}'(w_{0,r}^T x_i)w_r^T x_i = \text{relu}'(w_r^T x_i)w_r^T x_i - \text{relu}'(w_{0,r}^T x_i)w_r^T x_i \\
= \text{relu}'(w_r^T x_i)w_r^T x_i - \text{relu}'(w_{0,r}^T x_i)w_r^T x_i \\
+ \text{relu}'(w_{0,r}^T x_i)w_{0,r}^T x_i - \text{relu}'(w_{0,r}^T x_i)w_{0,r}^T x_i \\
= \text{relu}(w_r^T x_i) - \text{relu}(w_{0,r}^T x_i) + \text{relu}'(w_{0,r}^T x_i) (w_{0,r} - w_r, x_i) \\
\leq 2 \| w_r - w_{0,r} \|_2 \| x_i \|_2 \\
\leq 2 \omega M,
\]

where the last inequality holds for \( W \in \mathcal{W} \). It follows that

\[
\mathcal{R}_D(\mathcal{F}_{Q,M}) \leq \frac{1}{n} \mathbb{E} \left[ \sup_{W_0, v \in \mathcal{V}} \sum_{i=1}^{n} \epsilon_i \frac{1}{\sqrt{k}} \sum_{r=1}^{k} v_r \text{relu}'(w_{r,0}^T x_i)w_r^T x_i \right] \\
+ \frac{2M}{n \sqrt{k}} \sum_{i=1}^{n} \sum_{r=1}^{k} v_r \mathbb{1}_{\{\text{relu}'(w_{r,0}^T x_i) \neq \text{relu}'(w_r^T x_i)\}} \\
= \frac{1}{n} \mathbb{E} \left[ \epsilon^T \mathcal{J}_1(W_0, v) W \right] + \frac{2M}{n \sqrt{k}} \sum_{i=1}^{n} \sum_{r=1}^{k} v_r \mathbb{1}_{\{\text{relu}'(w_{r,0}^T x_i) \neq \text{relu}'(w_r^T x_i)\}} ,
\]

(56)
where $J_1$ is the Jacobian defined in (31), and where we use $v = \text{vect}(W) \in \mathbb{R}^{dk}$ for the vectorized version of the matrix $W$ with a slight abuse of notation. With this notation, we can bound the first term in (56) by

$$
\frac{1}{n} \mathbb{E} \left[ \sup_{\mathbf{w} \in W, \mathbf{v} \in V} \epsilon^T J_1(\mathbf{W}_0, \mathbf{v}) \mathbf{w} \right] = \frac{1}{n} \mathbb{E} \left[ \sup_{\mathbf{w} \in W, \mathbf{v} \in V} \epsilon^T (J_1(\mathbf{W}_0, \mathbf{v}) \mathbf{w} - J_1(\mathbf{W}_0, \mathbf{v}) \mathbf{w}_0) \right] \\
= \frac{1}{n} \mathbb{E} \left[ \sup_{\mathbf{w} \in W, \mathbf{v} \in V} \epsilon^T (J_1(\mathbf{W}_0, \mathbf{v})(\mathbf{w} - \mathbf{w}_0) + J_2(\mathbf{W}_0)(\mathbf{v} - \mathbf{v}_0)) \right] \\
= \frac{1}{n} \mathbb{E} \left[ \sup_{\mathbf{w} \in W, \mathbf{v} \in V} \epsilon^T (J_1(\mathbf{W}_0, \mathbf{v}_0)(\mathbf{w} - \mathbf{w}_0) + J_1(\mathbf{W}_0, \mathbf{v} - \mathbf{v}_0)(\mathbf{w} - \mathbf{w}_0) + J_2(\mathbf{W}_0)(\mathbf{v} - \mathbf{v}_0)) \right] \\
\leq \frac{1}{n} \mathbb{E} \left[ \|\epsilon^T J_1(\mathbf{W}_0, \mathbf{v}_0)\|_2 \right] Q + \frac{1}{n} \mathbb{E} \left[ \|\epsilon^T J_2(\mathbf{W}_0)\|_2 \right] Q + \sqrt{k} \nu \omega M^2 \tag{57}
$$

Here, equality (i) follows because $\epsilon J_1(\mathbf{W}_0, \mathbf{v}_0) \mathbf{w}_0$ has zero mean, inequality (ii) follows from the Cauchy-Schwarz inequality as well as from

$$
\|J_1(\mathbf{W}_0, \mathbf{v} - \mathbf{v}_0)(\mathbf{w} - \mathbf{w}_0)\|_2 \leq \frac{1}{\sqrt{k}} \|X\| \sum_{r=1}^k |v_r - v_{0,r}| \|\mathbf{w}_r - \mathbf{w}_{0,r}\|_2 \leq \sqrt{k} \nu \omega M^2 \sqrt{n},
$$

and inequality (iii) follows from $\mathbb{E} \left[ \|\mathbf{A}\|_2 \right] \leq \sqrt{\mathbb{E} \left[ \|\mathbf{A}\|^2 \right]} = \|\mathbf{A}\|_F$, by Jensen’s inequality, and from the bounds $\|J_1(\mathbf{W}_0, \mathbf{v}_0)\|_F \leq \nu$ and $\|J_2(\mathbf{W}_0)\|_F \leq \omega$, which holds with probability at least $1 - \delta$ provided that $\sqrt{\log(2n/\delta)}/2k \leq 1/2$, which in turn holds by assumption.

We next upper bound the second term in (56). Following the argument in [Aro+19, Proof of Lemma 5.4], we get

$$
\sum_{i=1}^n \sum_{r=1}^k v_r \mathbb{I}_{\{\text{relu}'(w_{i,o,x_i}) \neq \text{relu}'(w_{i,o,x_i})\}} \leq 2\nu kn \left( M + \sqrt{\frac{\log(2/\delta)}{2k}} \right), \tag{58}
$$

with probability at least $1 - \delta$. Here, we used that $v_r \leq |v_{0,r}| + |v_r - v_{0,r}| \leq 2\nu$. Putting the bounds on the first and second term in (56) (given by inequality (57) and inequality (58)) together, we get that, with probability at least $1 - \delta$, the Rademacher complexity is upper bounded by

$$
\mathcal{R}_D(\mathcal{F}) \leq \frac{Q}{\sqrt{n}}(\nu + \omega) + \omega \left( 5M^2 \sqrt{k} + 4M \sqrt{\log(2/\delta)} \right)
$$

which concludes our proof.